



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 9SOB / pdb\_00009sob  
EMDB ID : EMD-54657  
Title : Structural Model of the Nuclear Pore Complex in Arabidopsis thaliana  
Authors : Obarska-Kosinska, A.; Sanchez Carrillo, I.B.; Hoffmann, P.C.; Fourcassie, V.; Beck, M.; Germain, H.  
Deposited on : 2025-09-12  
Resolution : 35.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

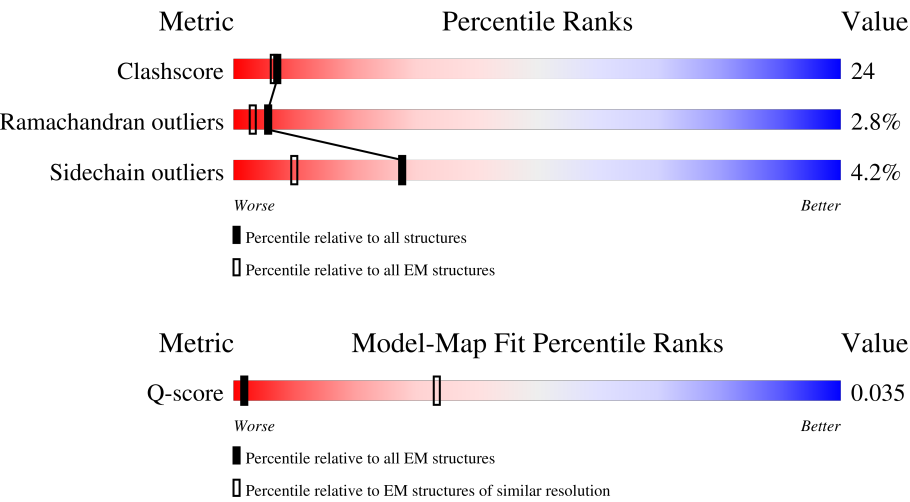
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 35.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 3 ( 33.00 - 33.00 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | R     | 1495   |                  |
| 1   | R16   | 1495   |                  |
| 1   | R8    | 1495   |                  |
| 2   | M     | 704    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | M16   | 704    |                  |
| 2   | M8    | 704    |                  |
| 3   | N     | 302    |                  |
| 3   | N16   | 302    |                  |
| 3   | N8    | 302    |                  |
| 4   | T     | 684    |                  |
| 4   | T16   | 684    |                  |
| 4   | T8    | 684    |                  |
| 5   | P     | 716    |                  |
| 5   | P16   | 716    |                  |
| 5   | P8    | 716    |                  |
| 6   | O     | 326    |                  |
| 6   | O16   | 326    |                  |
| 6   | O8    | 326    |                  |
| 7   | Q     | 361    |                  |
| 7   | Q16   | 361    |                  |
| 7   | Q8    | 361    |                  |
| 8   | L     | 977    |                  |
| 8   | L16   | 977    |                  |
| 8   | L8    | 977    |                  |
| 9   | K     | 709    |                  |
| 9   | K16   | 709    |                  |
| 9   | K8    | 709    |                  |
| 10  | C     | 1838   |                  |
| 10  | C16   | 1838   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10  | C24   | 1838   |                  |
| 10  | C32   | 1838   |                  |
| 10  | C8    | 1838   |                  |
| 11  | A16   | 860    |                  |
| 11  | A24   | 860    |                  |
| 11  | A32   | 860    |                  |
| 11  | A40   | 860    |                  |
| 12  | A     | 763    |                  |
| 12  | A48   | 763    |                  |
| 13  | V     | 196    |                  |
| 14  | W     | 810    |                  |
| 15  | J     | 185    |                  |
| 16  | A8    | 63     |                  |
| 17  | F     | 28     |                  |
| 17  | F16   | 28     |                  |
| 17  | F24   | 28     |                  |
| 17  | F8    | 28     |                  |
| 18  | B     | 1965   |                  |
| 18  | B8    | 1965   |                  |
| 19  | 4     | 447    |                  |
| 19  | 48    | 447    |                  |
| 20  | E     | 519    |                  |
| 20  | E8    | 519    |                  |
| 21  | H     | 254    |                  |
| 21  | H16   | 254    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 21  | H24   | 254    |                  |
| 21  | H8    | 254    |                  |
| 22  | I     | 237    |                  |
| 22  | I16   | 237    |                  |
| 22  | I24   | 237    |                  |
| 22  | I8    | 237    |                  |
| 23  | J16   | 197    |                  |
| 23  | J24   | 197    |                  |
| 23  | J32   | 197    |                  |
| 23  | J8    | 197    |                  |
| 24  | D     | 1464   |                  |
| 24  | D16   | 1464   |                  |
| 24  | D24   | 1464   |                  |
| 24  | D32   | 1464   |                  |
| 24  | D40   | 1464   |                  |
| 24  | D8    | 1464   |                  |

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 402561 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nuclear pore complex protein NUP160.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | R     | 1464     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11593 | 7388 | 1952 | 2188 | 65 |         |       |
| 1   | R8    | 1464     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11593 | 7388 | 1952 | 2188 | 65 |         |       |
| 1   | R16   | 1464     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11593 | 7388 | 1952 | 2188 | 65 |         |       |

- Molecule 2 is a protein called Nuclear pore complex protein NUP96.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | M     | 696      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5598  | 3577 | 939 | 1054 | 28 |         |       |
| 2   | M8    | 696      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5598  | 3577 | 939 | 1054 | 28 |         |       |
| 2   | M16   | 696      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5598  | 3577 | 939 | 1054 | 28 |         |       |

- Molecule 3 is a protein called Protein transport protein SEC13 homolog B.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | N     | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2302  | 1451 | 398 | 444 | 9 |         |       |
| 3   | N8    | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2302  | 1451 | 398 | 444 | 9 |         |       |
| 3   | N16   | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2302  | 1451 | 398 | 444 | 9 |         |       |

- Molecule 4 is a protein called E3 ubiquitin-protein ligase HOS1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 4   | T     | 684      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5498  | 3453 | 960 | 1049 | 36 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 4   | T8    | 684      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5498  | 3453 | 960 | 1049 | 36 |         |       |
| 4   | T16   | 684      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5498  | 3453 | 960 | 1049 | 36 |         |       |

- Molecule 5 is a protein called Nuclear pore complex protein NUP85.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 5   | P     | 708      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5620  | 3572 | 974 | 1041 | 33 |         |       |
| 5   | P8    | 708      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5620  | 3572 | 974 | 1041 | 33 |         |       |
| 5   | P16   | 708      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5620  | 3572 | 974 | 1041 | 33 |         |       |

- Molecule 6 is a protein called Protein SEH1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | O     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2336  | 1467 | 387 | 468 | 14 |         |       |
| 6   | O8    | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2336  | 1467 | 387 | 468 | 14 |         |       |
| 6   | O16   | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2336  | 1467 | 387 | 468 | 14 |         |       |

- Molecule 7 is a protein called Nuclear pore complex protein NUP43.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | Q     | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2770  | 1732 | 480 | 546 | 12 |         |       |
| 7   | Q8    | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2770  | 1732 | 480 | 546 | 12 |         |       |
| 7   | Q16   | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2770  | 1732 | 480 | 546 | 12 |         |       |

- Molecule 8 is a protein called Nuclear pore complex protein NUP107.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 8   | L     | 974      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7770  | 4912 | 1322 | 1481 | 55 |         |       |
| 8   | L8    | 974      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7770  | 4912 | 1322 | 1481 | 55 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 8   | L16   | 974      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7770  | 4912 | 1322 | 1481 | 55 |         |       |

- Molecule 9 is a protein called Nuclear pore complex protein NUP133.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 9   | K     | 705      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5695  | 3569 | 992 | 1104 | 30 |         |       |
| 9   | K8    | 705      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5695  | 3569 | 992 | 1104 | 30 |         |       |
| 9   | K16   | 705      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5696  | 3569 | 992 | 1105 | 30 |         |       |

- Molecule 10 is a protein called Nuclear pore complex protein NUP205.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 10  | C16   | 1838     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 14529 | 9239 | 2457 | 2763 | 70 |         |       |
| 10  | C24   | 1838     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 14529 | 9239 | 2457 | 2763 | 70 |         |       |
| 10  | C     | 1824     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 14402 | 9155 | 2437 | 2740 | 70 |         |       |
| 10  | C8    | 1793     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 14177 | 9023 | 2397 | 2687 | 70 |         |       |
| 10  | C32   | 1838     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 14529 | 9239 | 2457 | 2763 | 70 |         |       |

- Molecule 11 is a protein called Nuclear pore complex protein NUP93A.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11  | A24   | 818      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6472  | 4058 | 1154 | 1227 | 33 |         |       |
| 11  | A40   | 818      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6472  | 4058 | 1154 | 1227 | 33 |         |       |
| 11  | A16   | 818      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6472  | 4058 | 1154 | 1227 | 33 |         |       |
| 11  | A32   | 818      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6472  | 4058 | 1154 | 1227 | 33 |         |       |

- Molecule 12 is a protein called Nuclear pore complex protein NUP93A.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 12  | A     | 723      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5726  | 3594 | 1023 | 1078 | 31 |         |       |
| 12  | A48   | 726      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5752  | 3612 | 1026 | 1083 | 31 |         |       |

- Molecule 13 is a protein called Nuclear pore complex protein NUP214.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 13  | V     | 196      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1590  | 987 | 289 | 304 | 10 |         |       |

- Molecule 14 is a protein called Nuclear pore complex protein NUP88.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 14  | W     | 787      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6141  | 3886 | 1047 | 1185 | 23 |         |       |

- Molecule 15 is a protein called Nuclear pore complex protein NUP62.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | J     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1504  | 923 | 266 | 310 | 5 |         |       |

- Molecule 16 is a protein called Nuclear pore complex protein NUP93A.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 16  | A8    | 63       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 523   | 326 | 90 | 102 | 5 |         |       |

- Molecule 17 is a protein called Nuclear pore complex protein NUP35.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | F8    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 213   | 133 | 31 | 48 | 1 |         |       |
| 17  | F     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 213   | 133 | 31 | 48 | 1 |         |       |
| 17  | F24   | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 213   | 133 | 31 | 48 | 1 |         |       |
| 17  | F16   | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 213   | 133 | 31 | 48 | 1 |         |       |

- Molecule 18 is a protein called Nucleoporin (DUF3414).

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 18  | B     | 1965     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15417 | 9887 | 2528 | 2913 | 89 |         |       |
| 18  | B8    | 1965     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 15417 | 9887 | 2528 | 2913 | 89 |         |       |

- Molecule 19 is a protein called Aladin.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | 4     | 447      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3413  | 2155 | 583 | 659 | 16 |         |       |
| 19  | 48    | 447      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3413  | 2155 | 583 | 659 | 16 |         |       |

- Molecule 20 is a protein called Nucleoporin protein Ndc1-Nup protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | E     | 519      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4057  | 2648 | 667 | 727 | 15 |         |       |
| 20  | E8    | 519      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4057  | 2648 | 667 | 727 | 15 |         |       |

- Molecule 21 is a protein called Nuclear pore complex protein NUP54.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | H     | 254      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2023  | 1254 | 366 | 392 | 11 |         |       |
| 21  | H8    | 254      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2023  | 1254 | 366 | 392 | 11 |         |       |
| 21  | H24   | 254      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2023  | 1254 | 366 | 392 | 11 |         |       |
| 21  | H16   | 254      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2023  | 1254 | 366 | 392 | 11 |         |       |

- Molecule 22 is a protein called NUP58.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | I     | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1939  | 1219 | 351 | 359 | 10 |         |       |
| 22  | I8    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1939  | 1219 | 351 | 359 | 10 |         |       |
| 22  | I24   | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1939  | 1219 | 351 | 359 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | I16   | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1939  | 1219 | 351 | 359 | 10 |         |       |

- Molecule 23 is a protein called Nuclear pore complex protein NUP62.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | J32   | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1601  | 983 | 284 | 327 | 7 |         |       |
| 23  | J8    | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1601  | 983 | 284 | 327 | 7 |         |       |
| 23  | J24   | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1601  | 983 | 284 | 327 | 7 |         |       |
| 23  | J16   | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1601  | 983 | 284 | 327 | 7 |         |       |

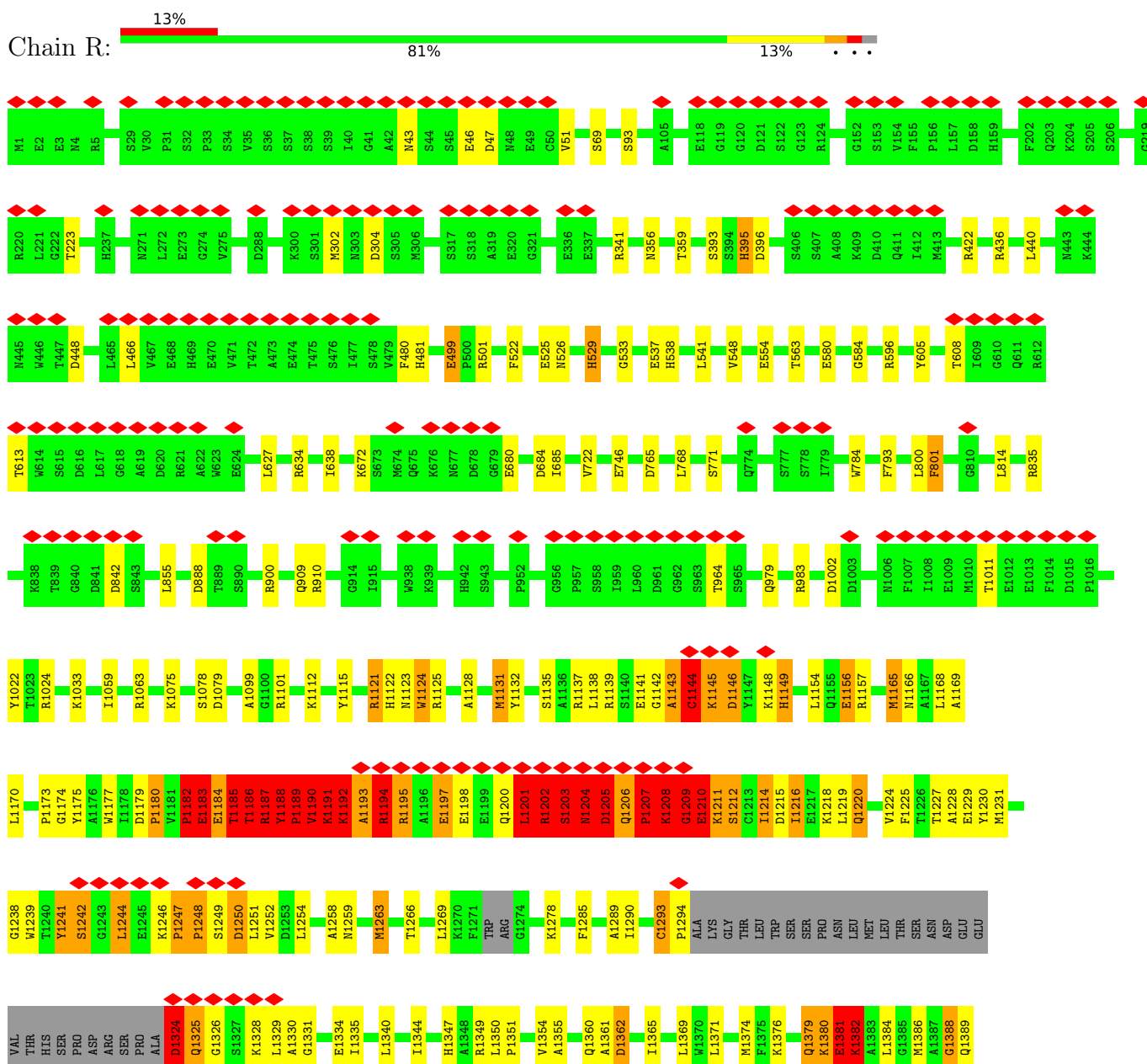
- Molecule 24 is a protein called Nuclear pore complex protein NUP155.

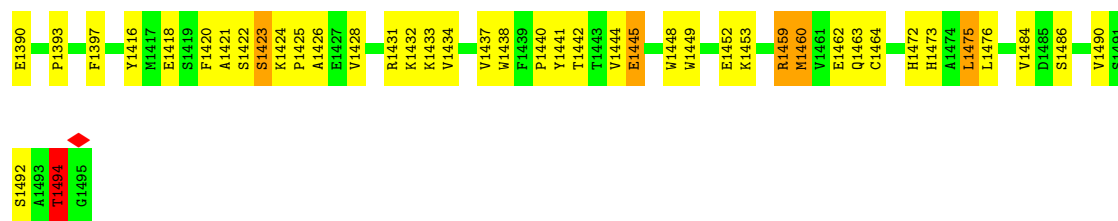
| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 24  | D     | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |
| 24  | D8    | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |
| 24  | D16   | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |
| 24  | D24   | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |
| 24  | D32   | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |
| 24  | D40   | 1453     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11141 | 6950 | 1960 | 2168 | 63 |         |       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

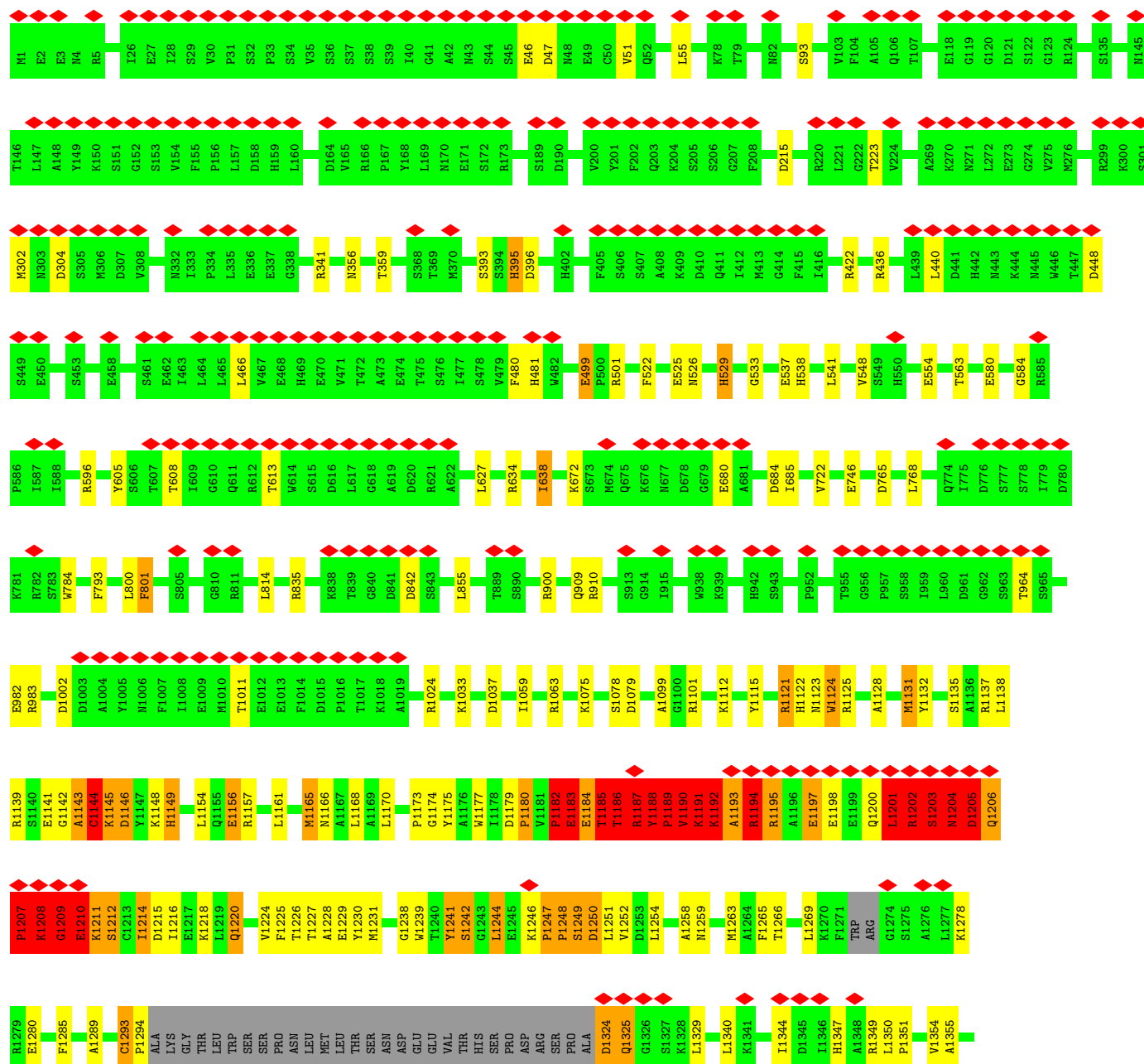
- Molecule 1: Nuclear pore complex protein NUP160

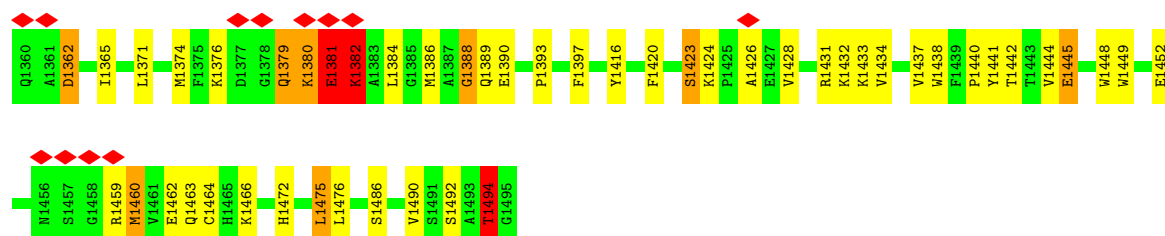




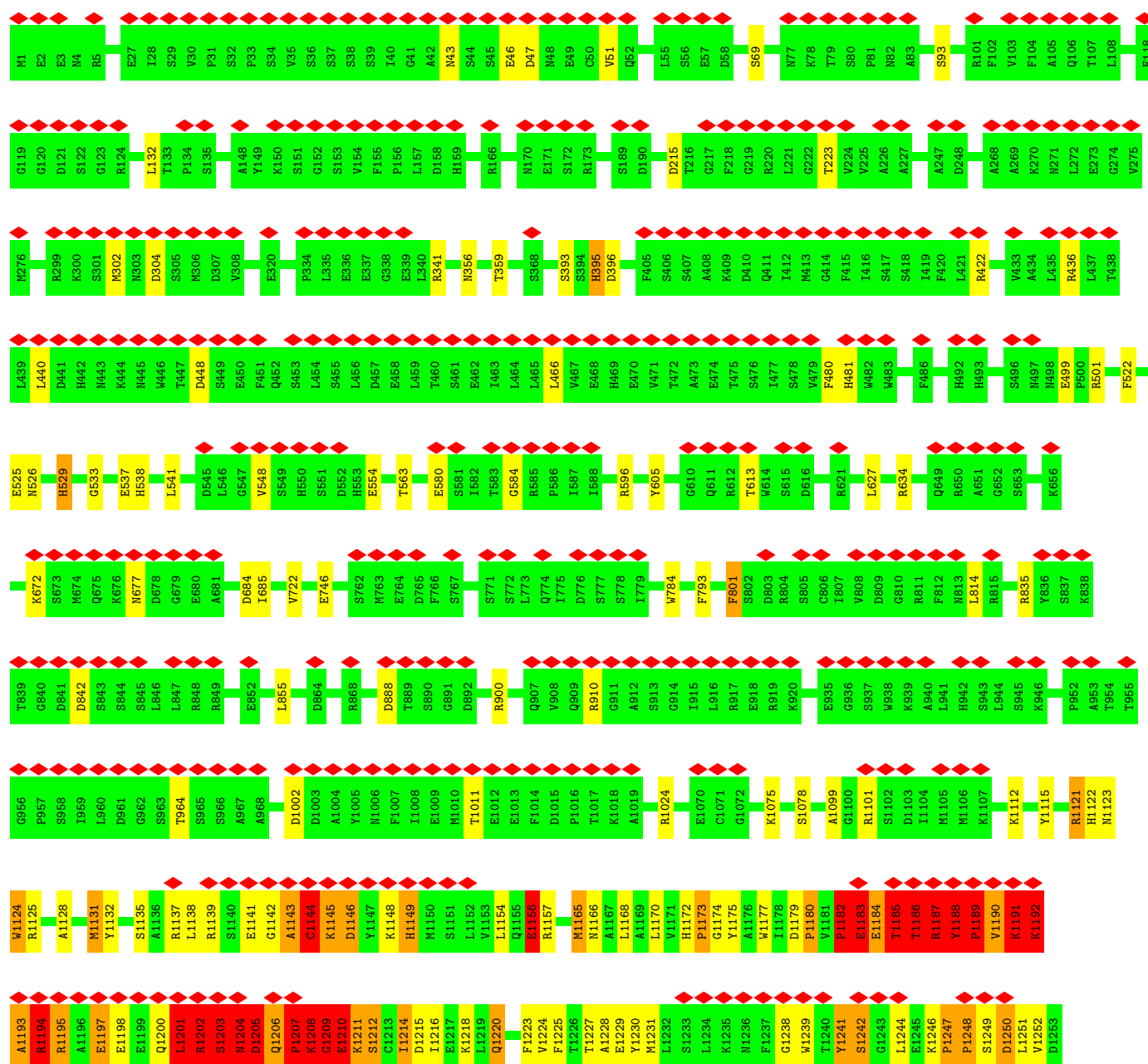
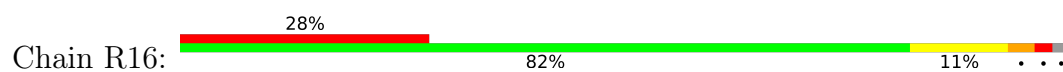
• Molecule 1: Nuclear pore complex protein NUP160

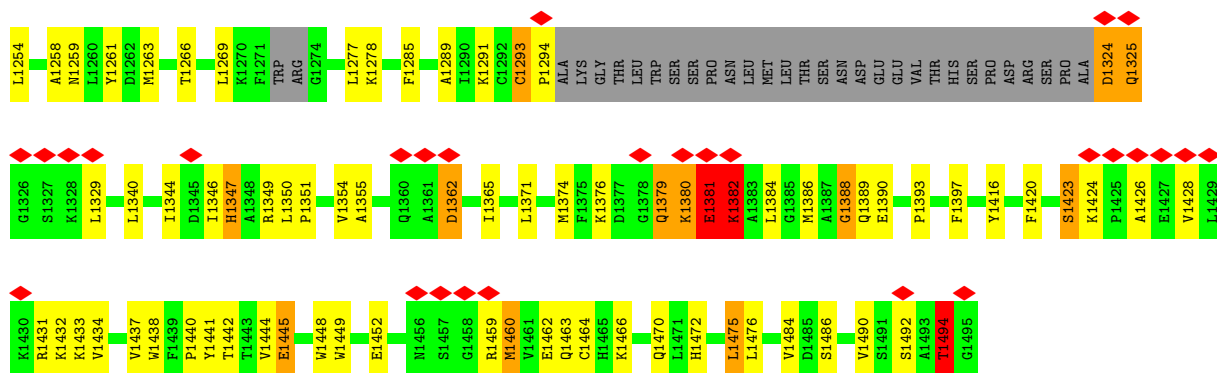
Chain R8: 19% 82% 12% . . .



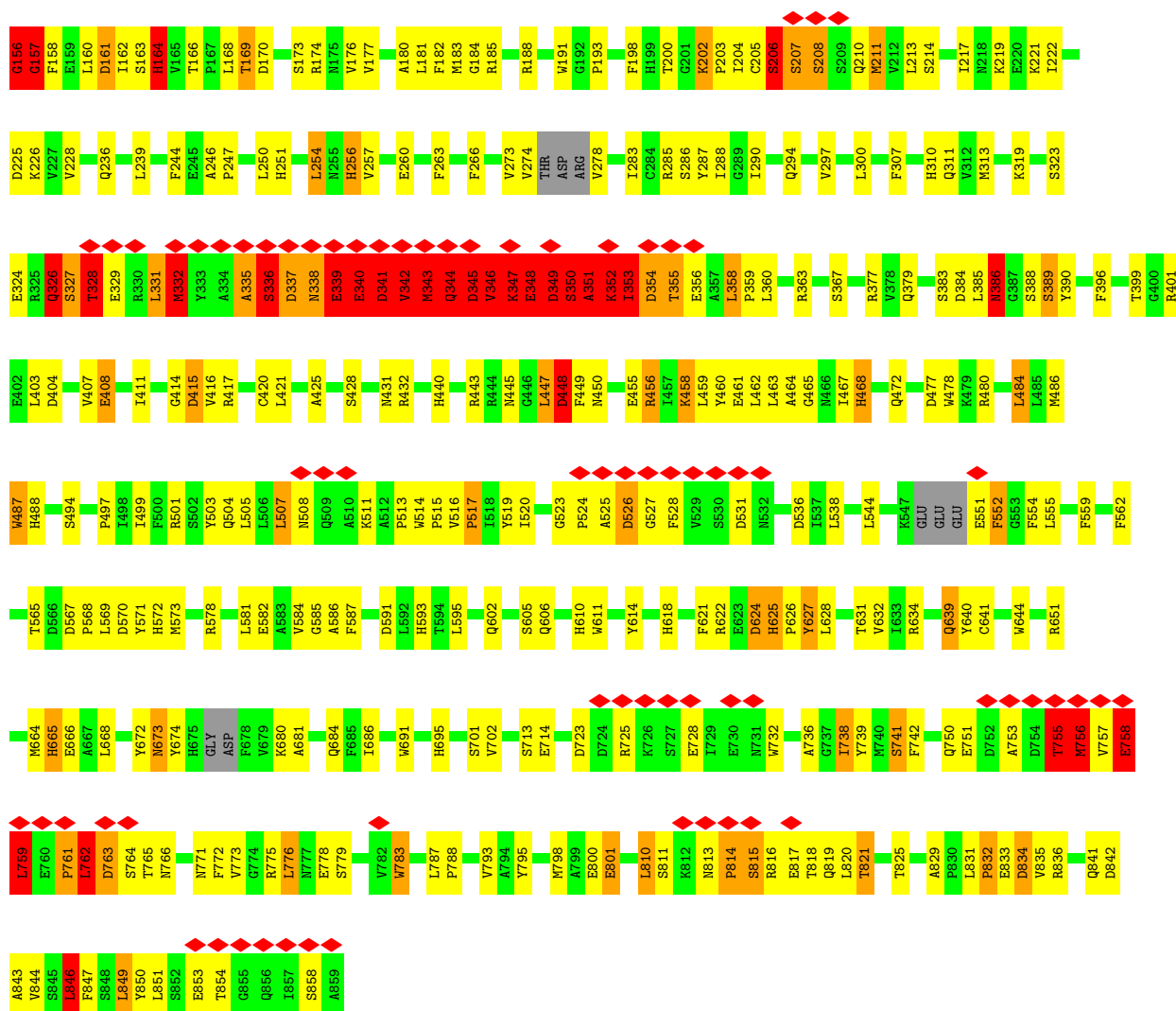


• Molecule 1: Nuclear pore complex protein NUP160





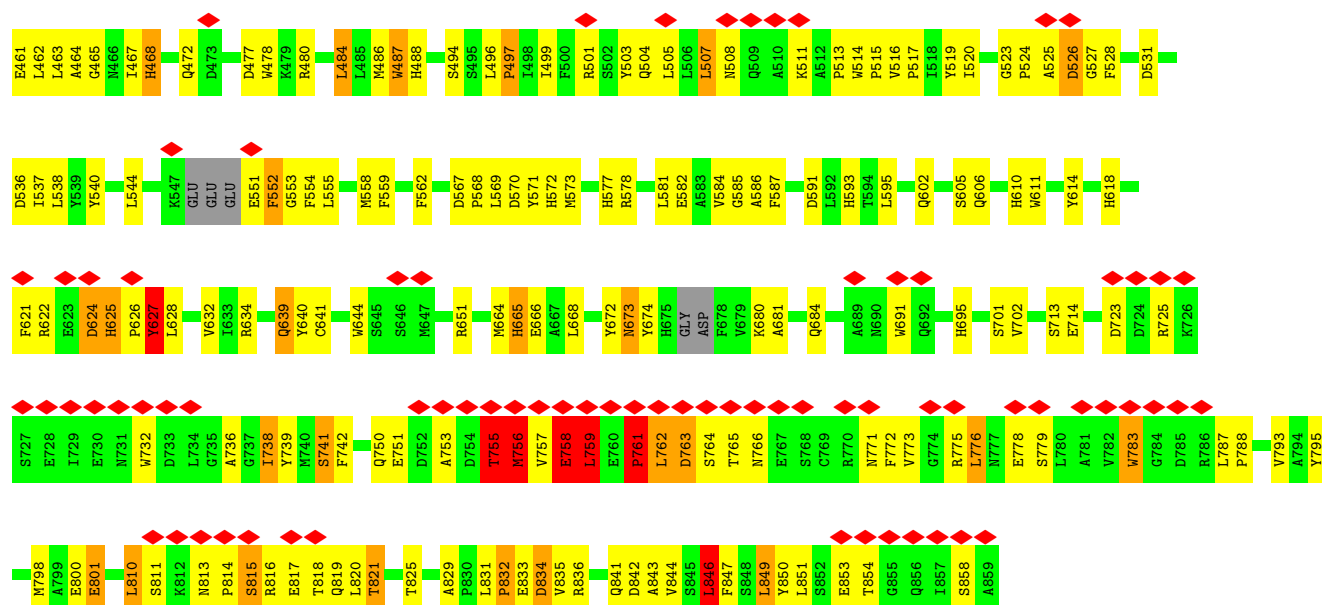
• Molecule 2: Nuclear pore complex protein NUP96



• Molecule 2: Nuclear pore complex protein NUP96

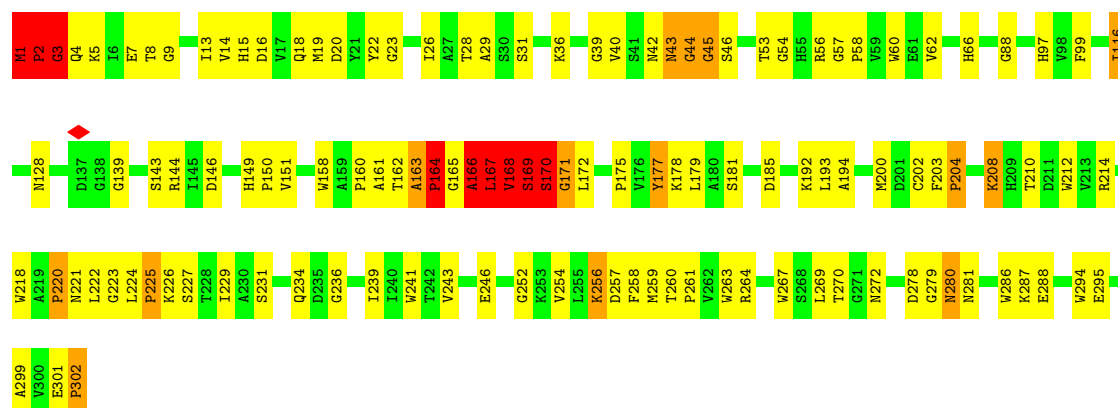






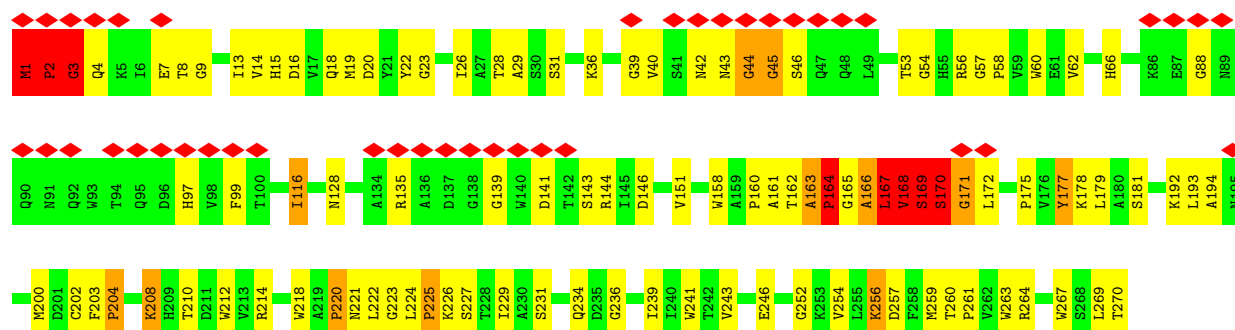
• Molecule 3: Protein transport protein SEC13 homolog B

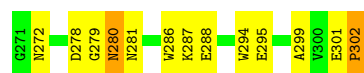
Chain N: 59% 33% 5%



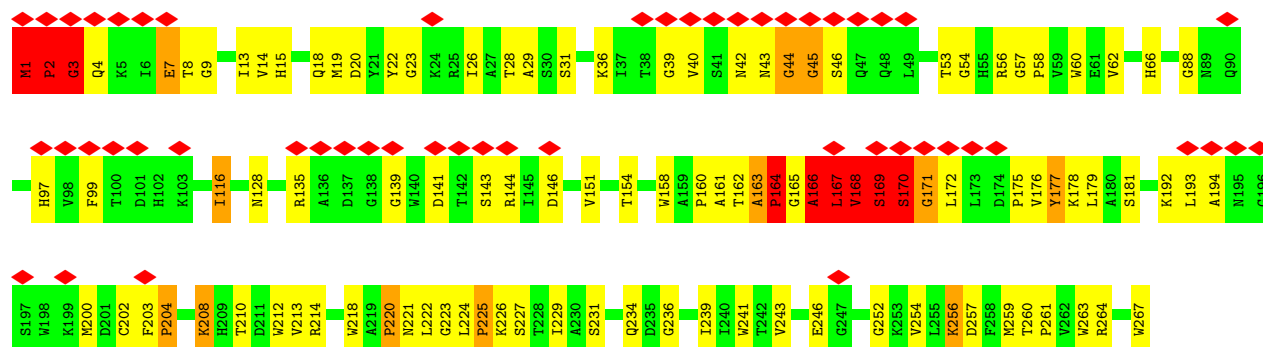
• Molecule 3: Protein transport protein SEC13 homolog B

Chain N8: 14% 60% 32% 5%

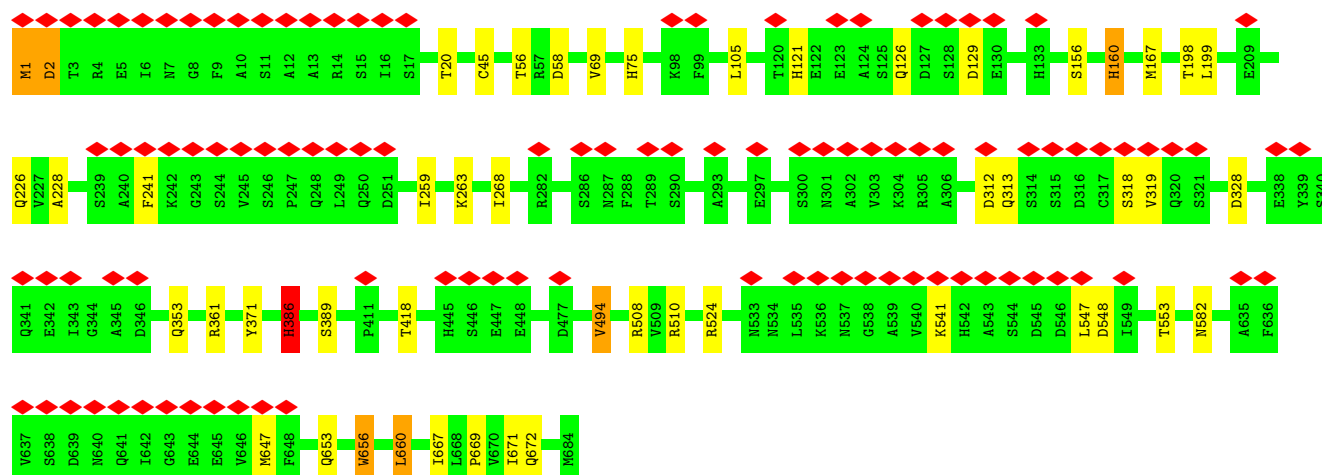




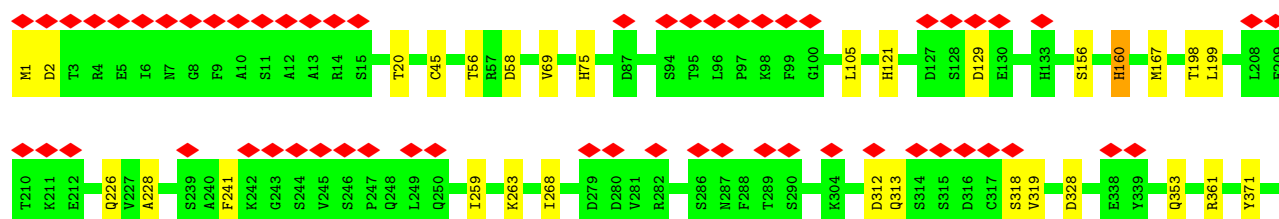
• Molecule 3: Protein transport protein SEC13 homolog B

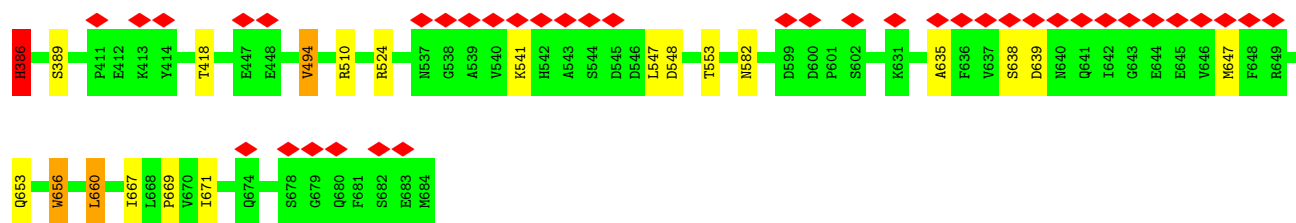


• Molecule 4: E3 ubiquitin-protein ligase HOS1

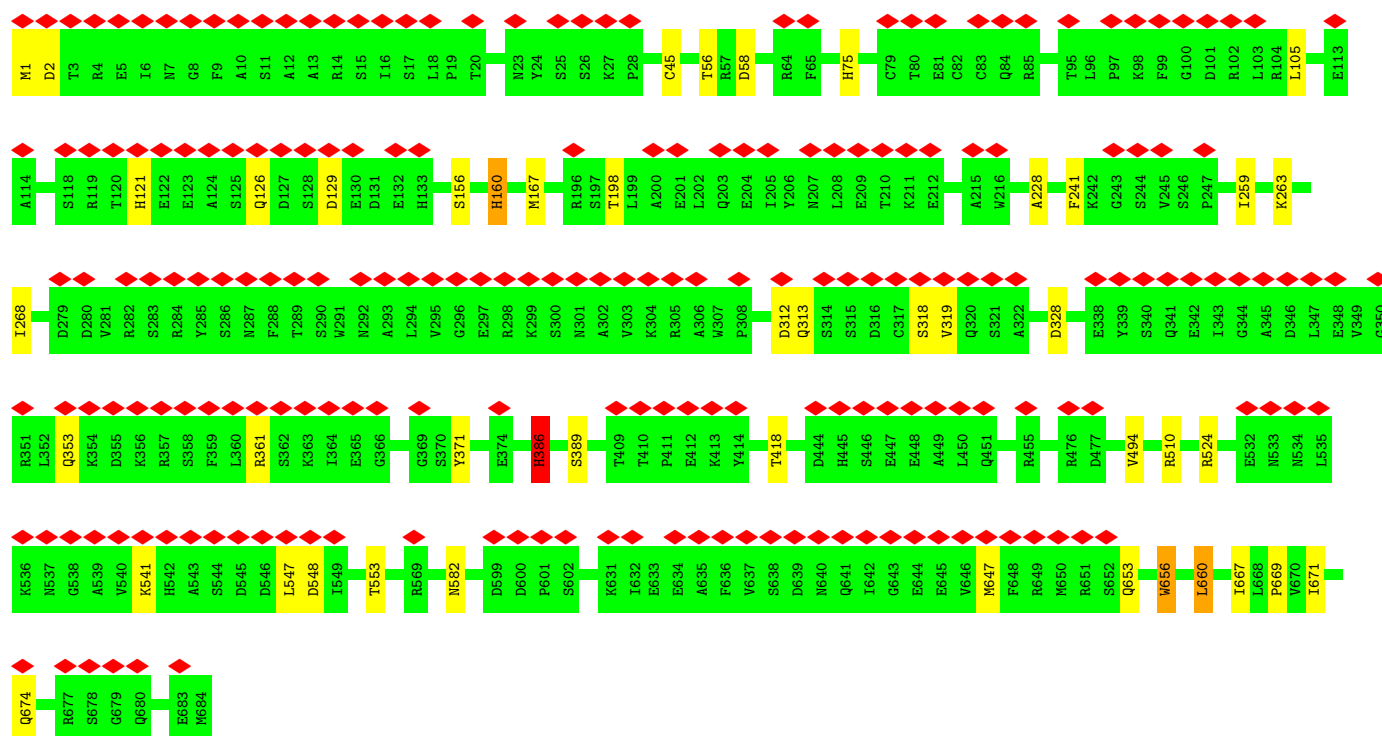


• Molecule 4: E3 ubiquitin-protein ligase HOS1

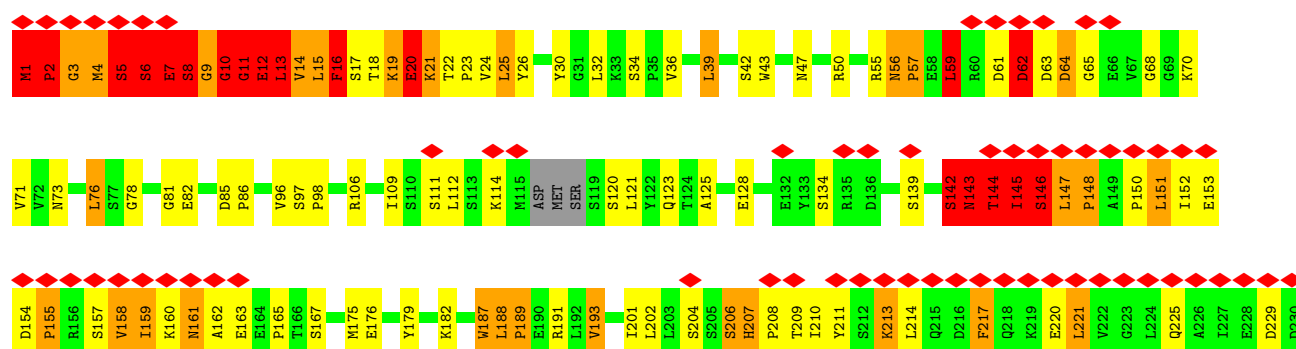


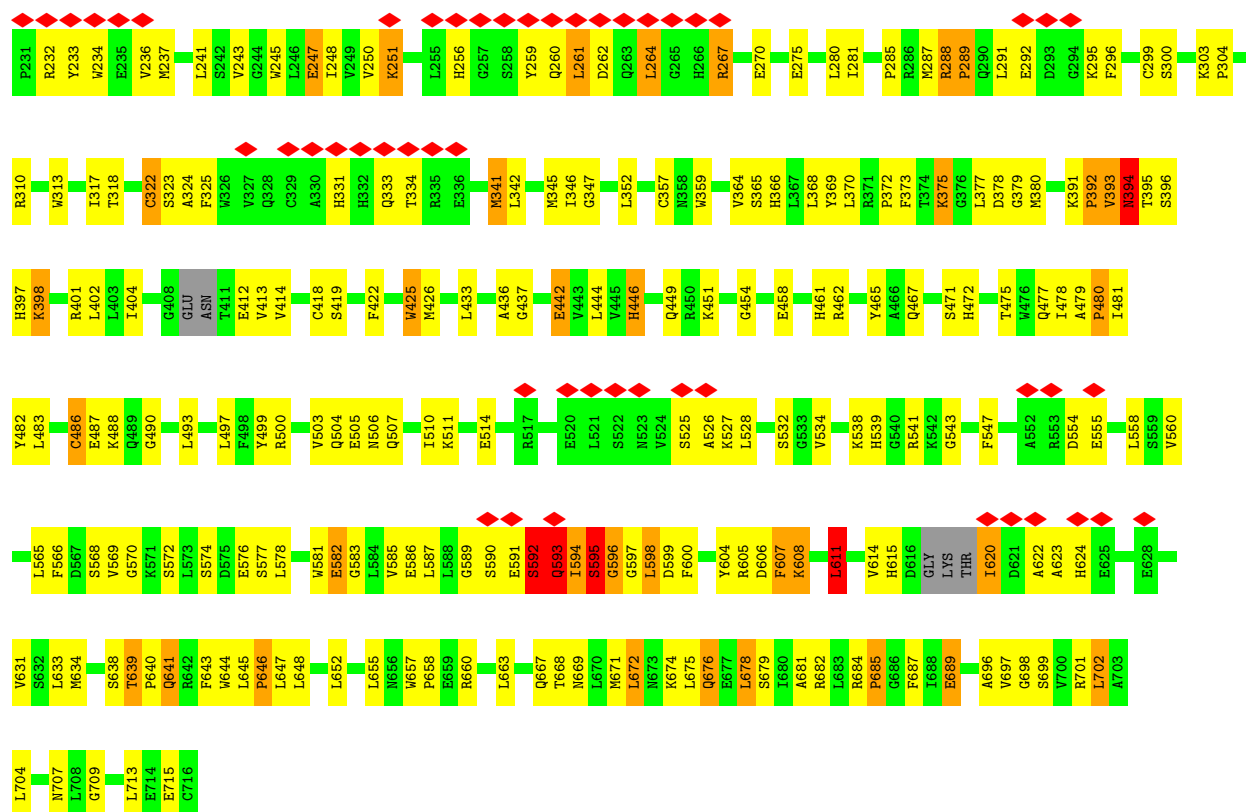


• Molecule 4: E3 ubiquitin-protein ligase HOS1

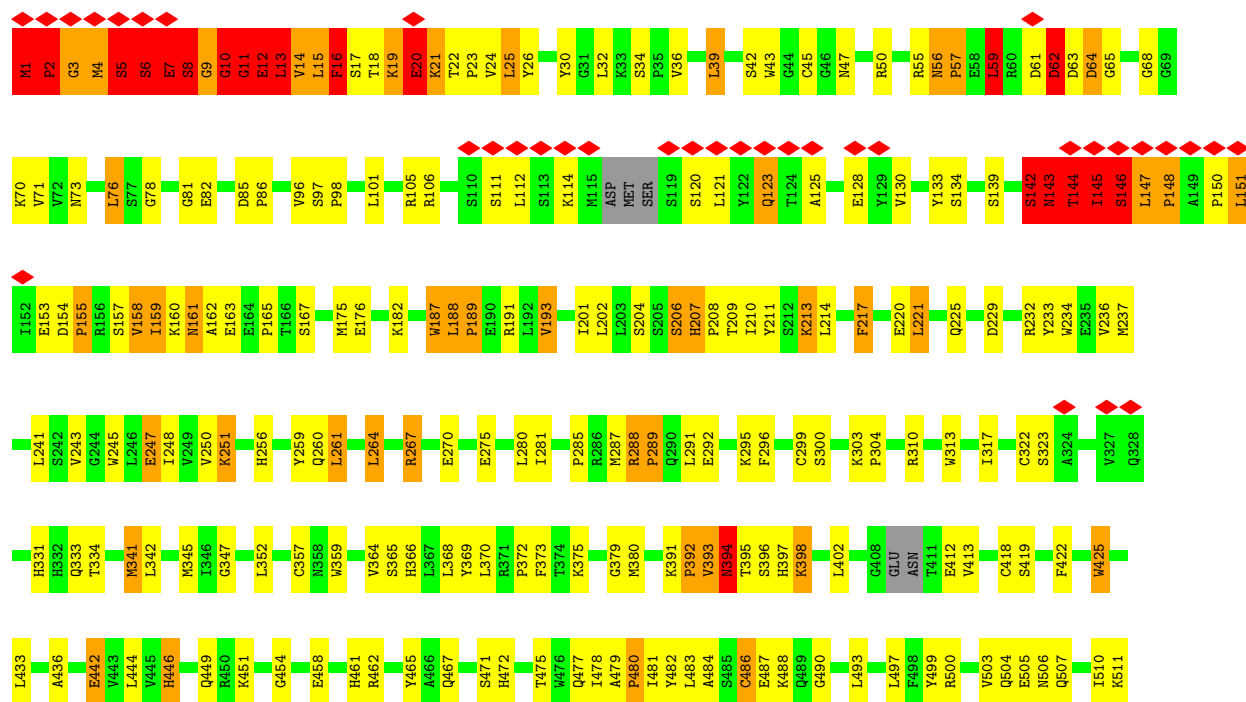


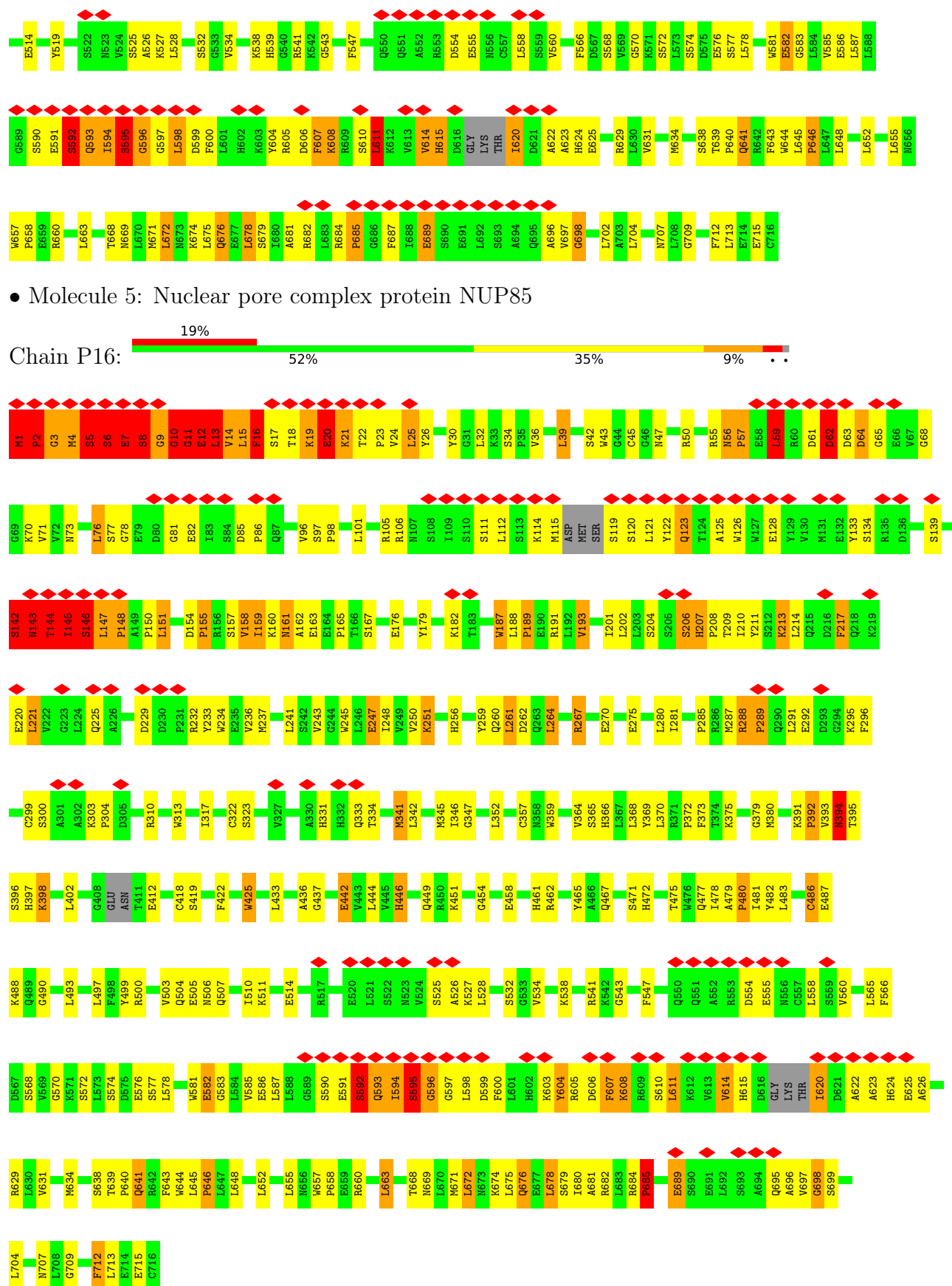
• Molecule 5: Nuclear pore complex protein NUP85



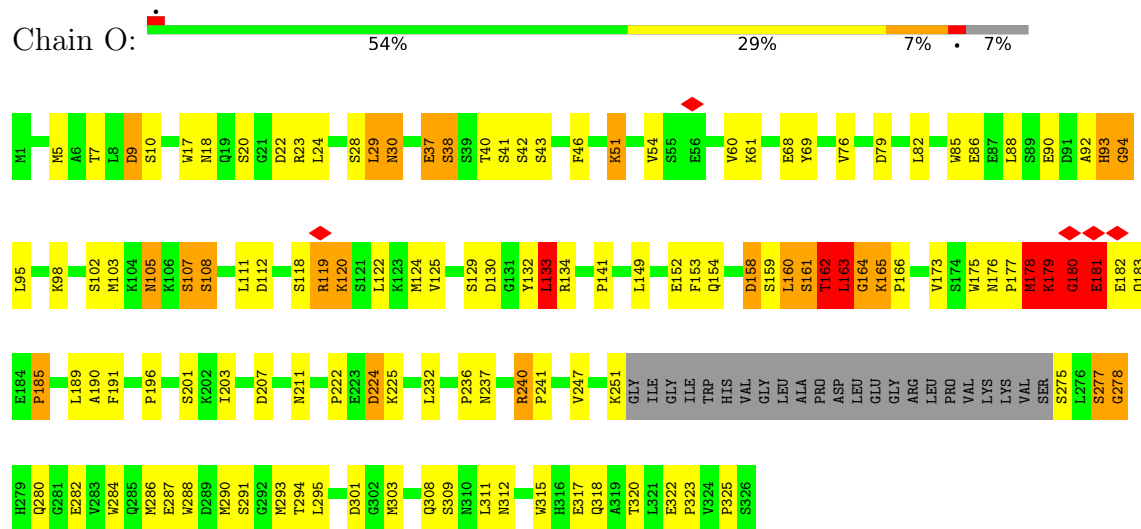


• Molecule 5: Nuclear pore complex protein NUP85

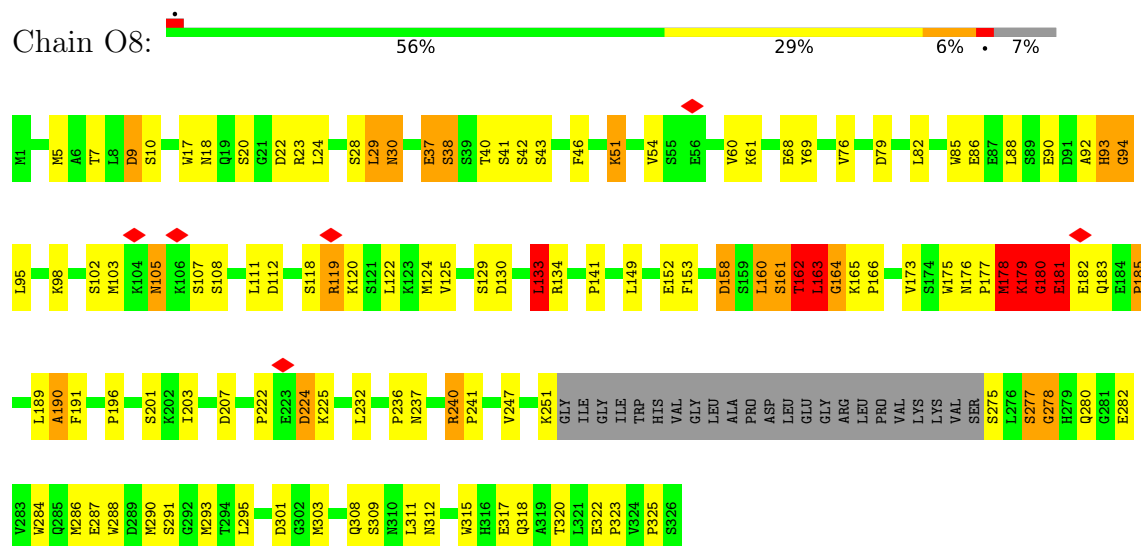




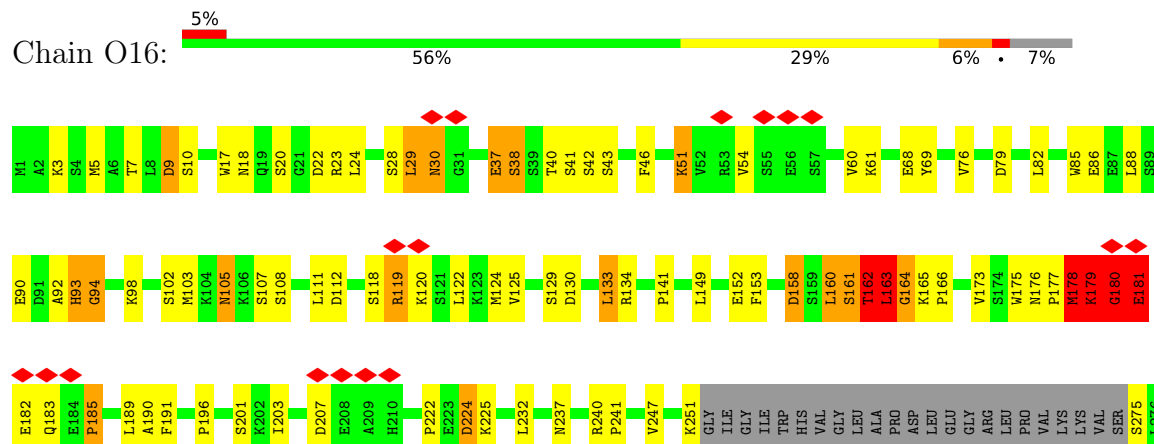
• Molecule 6: Protein SEH1



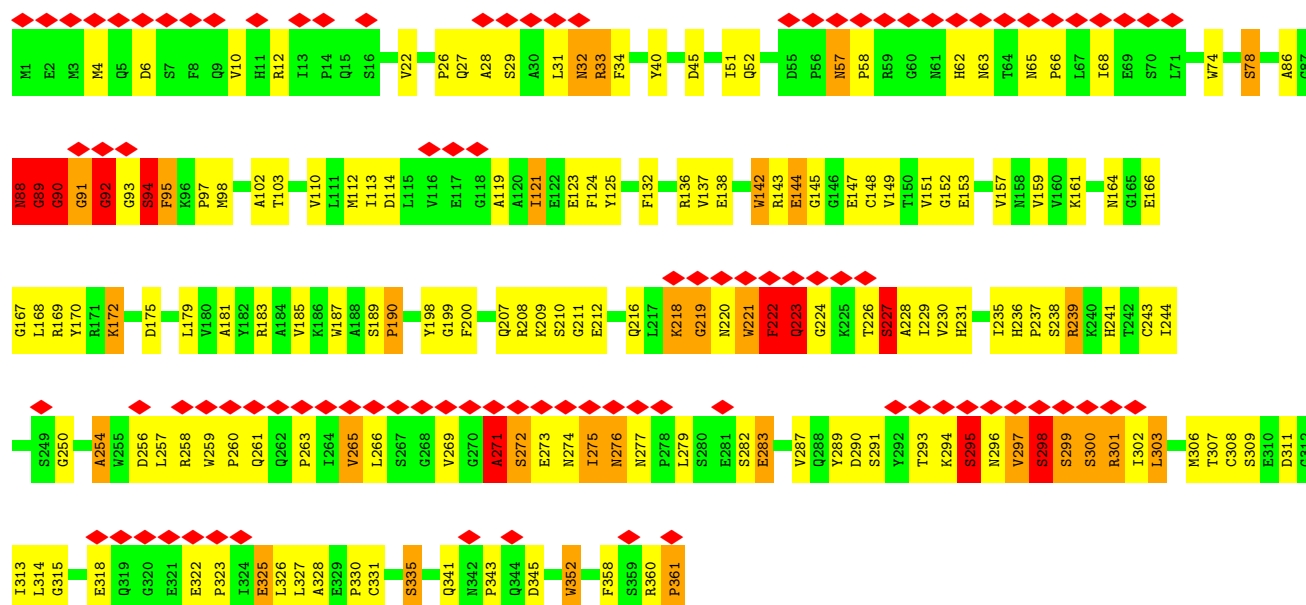
• Molecule 6: Protein SEH1



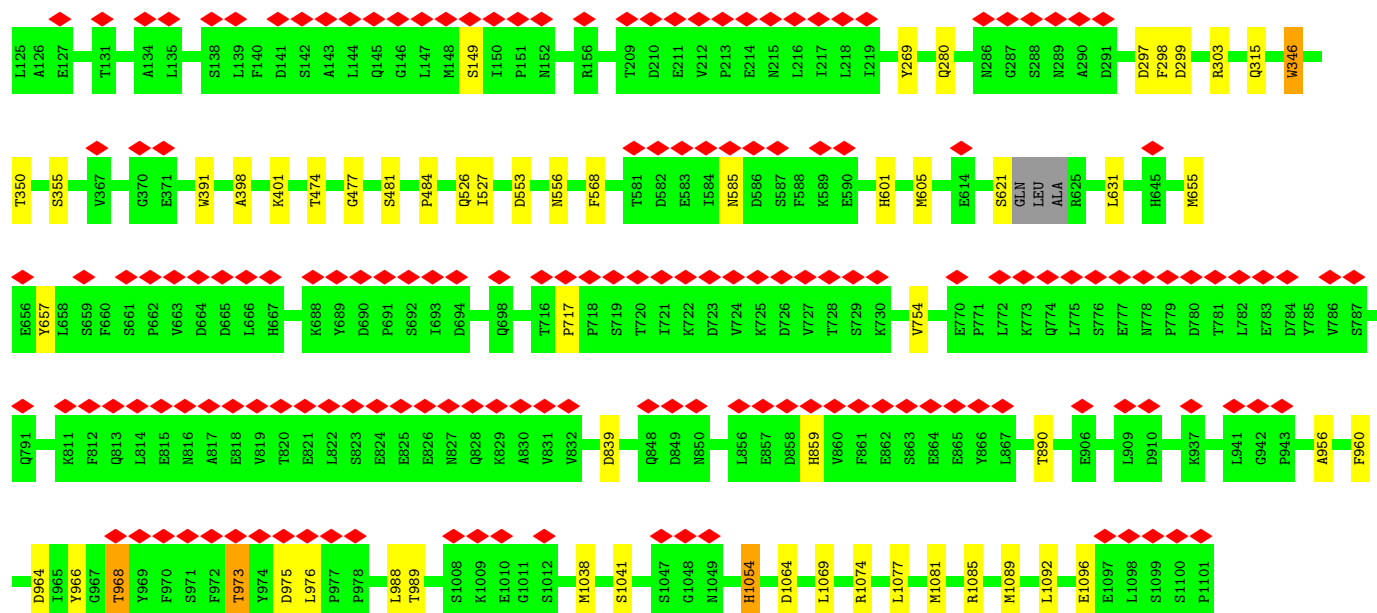
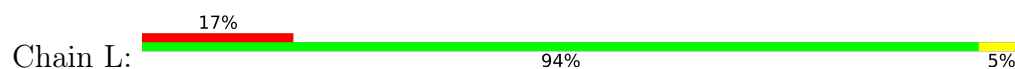
• Molecule 6: Protein SEH1



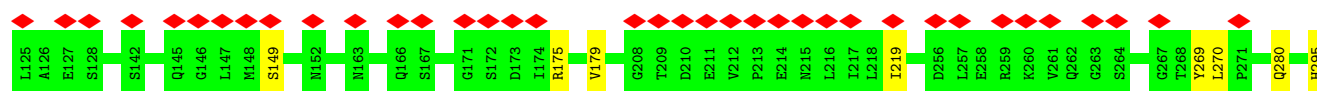


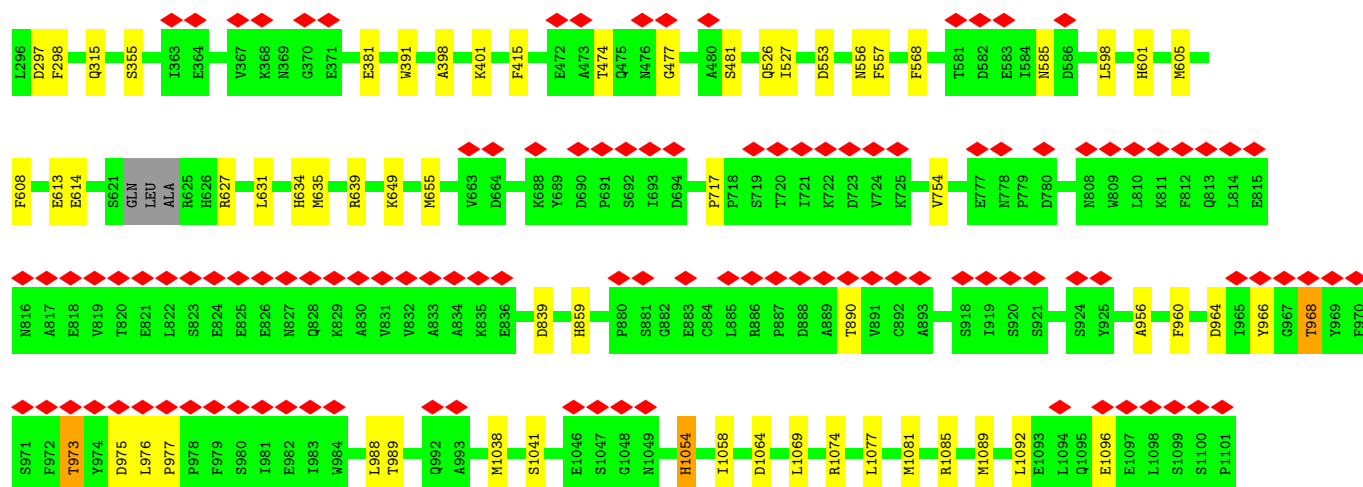


• Molecule 8: Nuclear pore complex protein NUP107

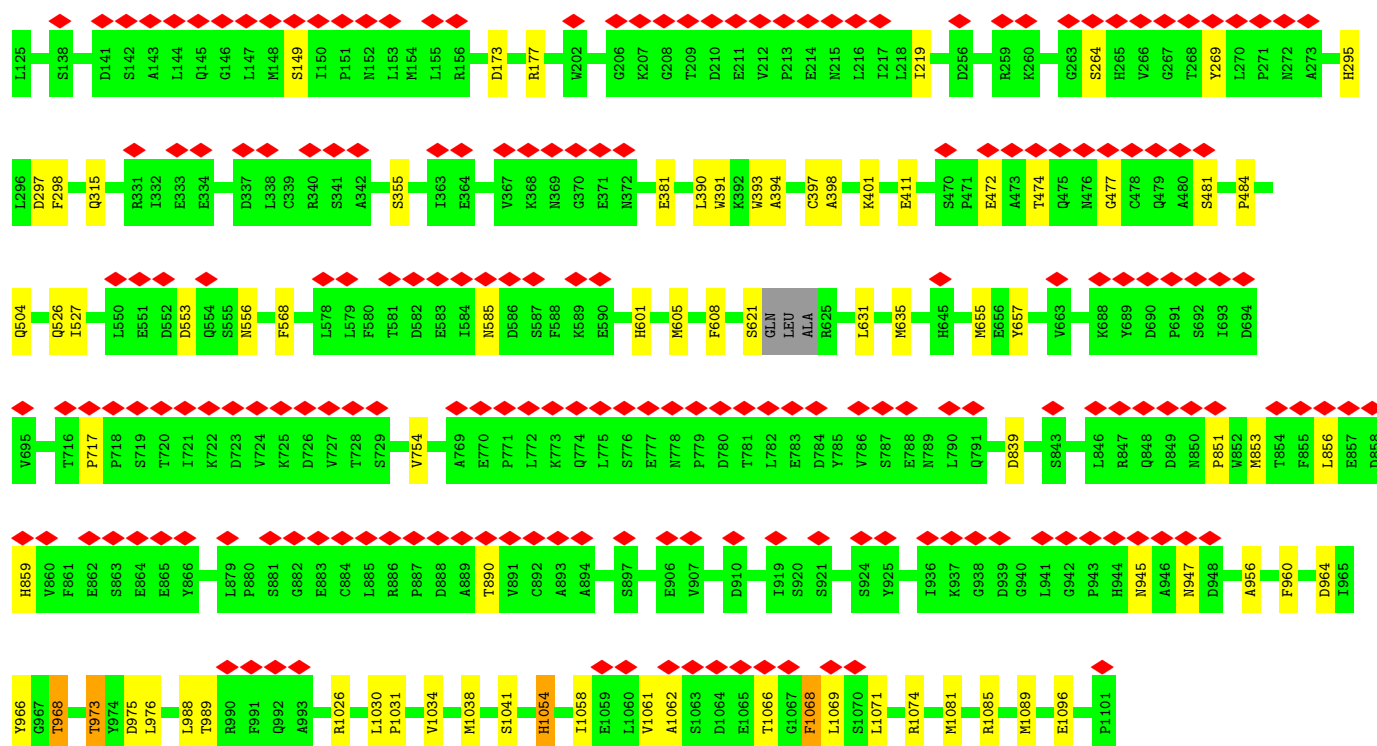


• Molecule 8: Nuclear pore complex protein NUP107

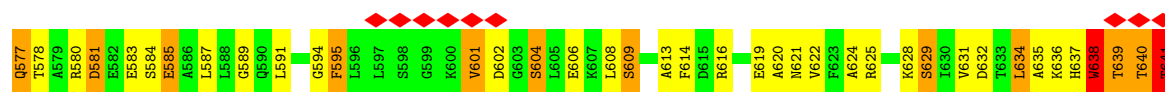


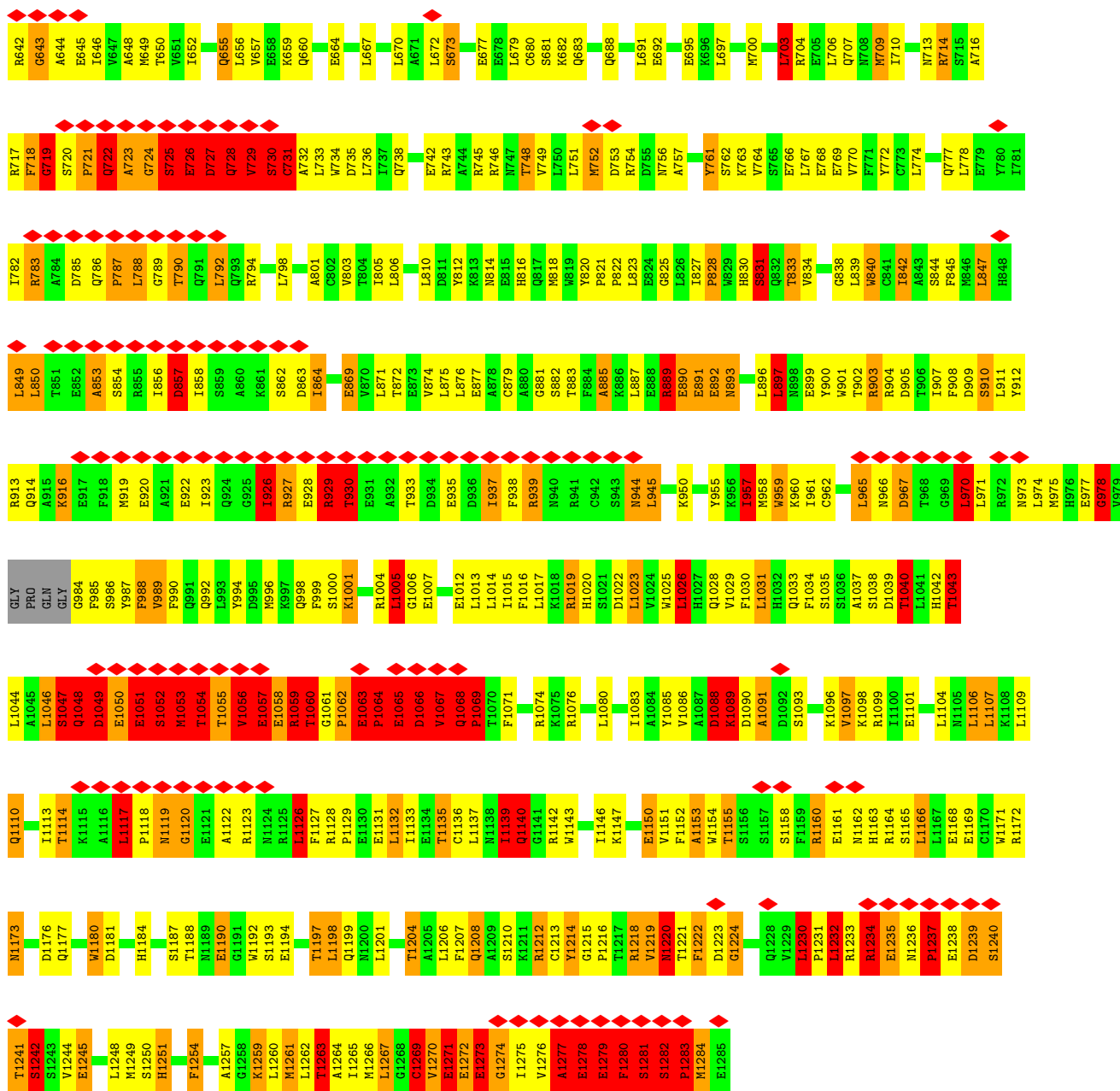


• Molecule 8: Nuclear pore complex protein NUP107



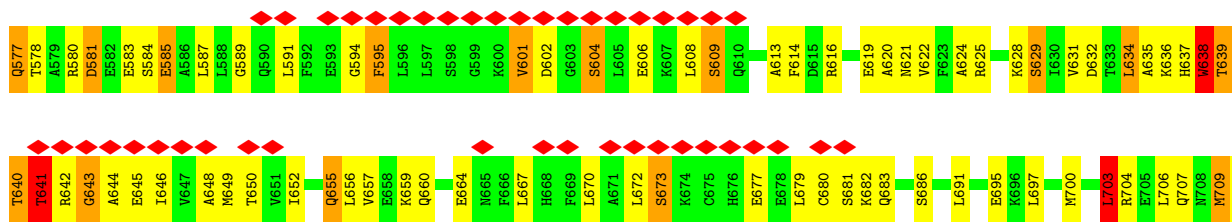
• Molecule 9: Nuclear pore complex protein NUP133



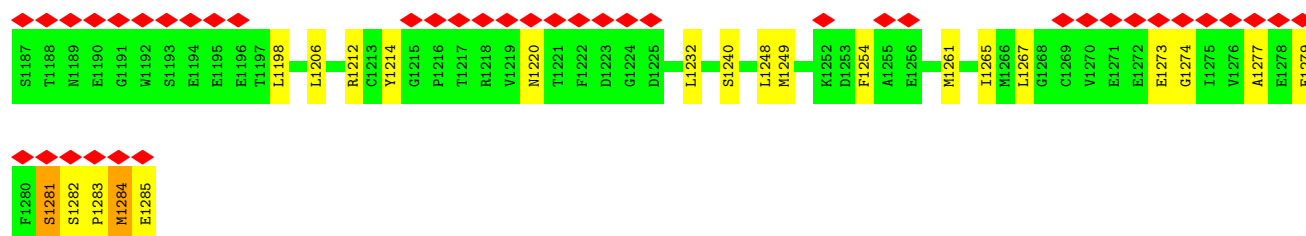


• Molecule 9: Nuclear pore complex protein NUP133

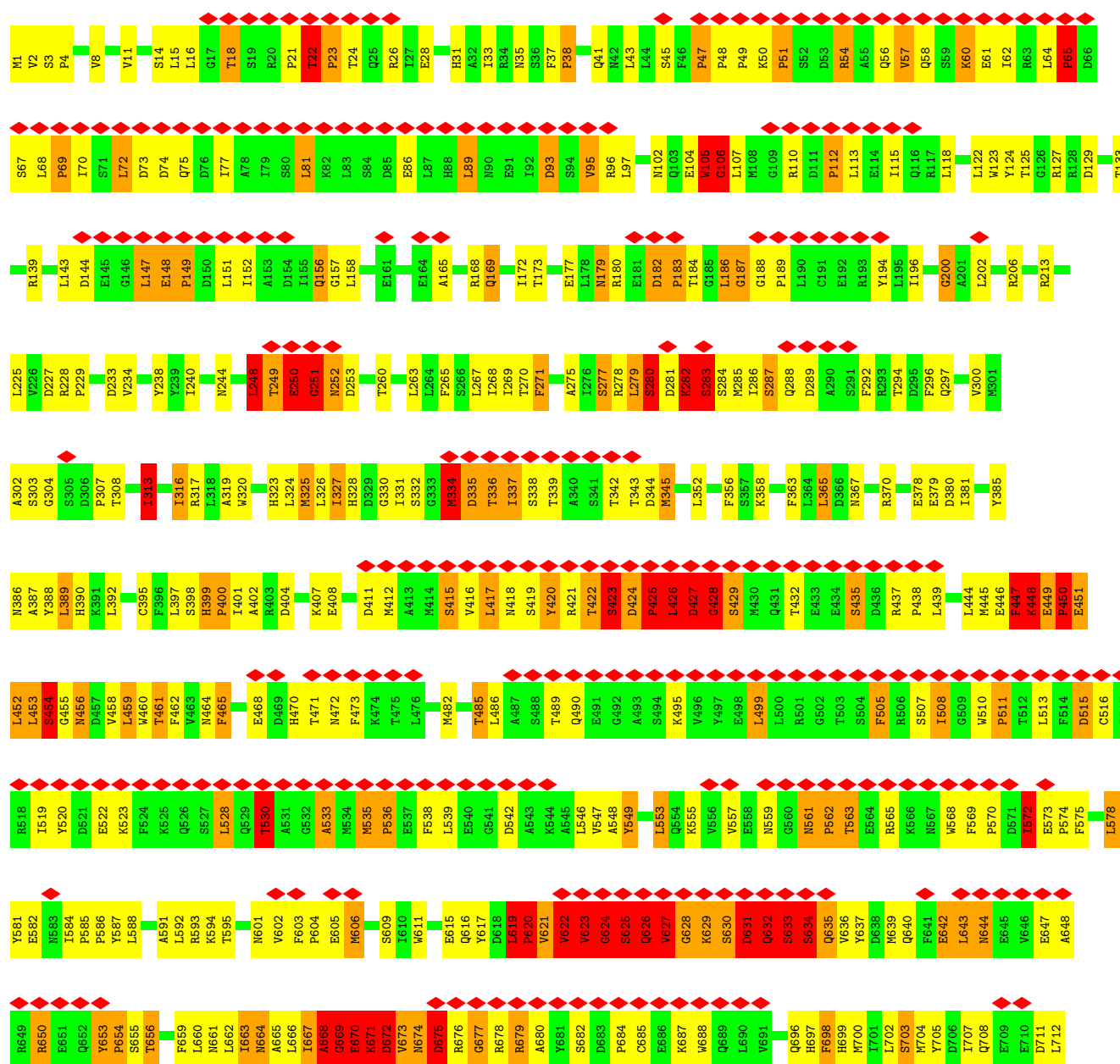
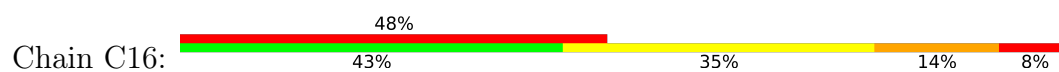
Chain K8: 36% 36% 38% 16% 9%.



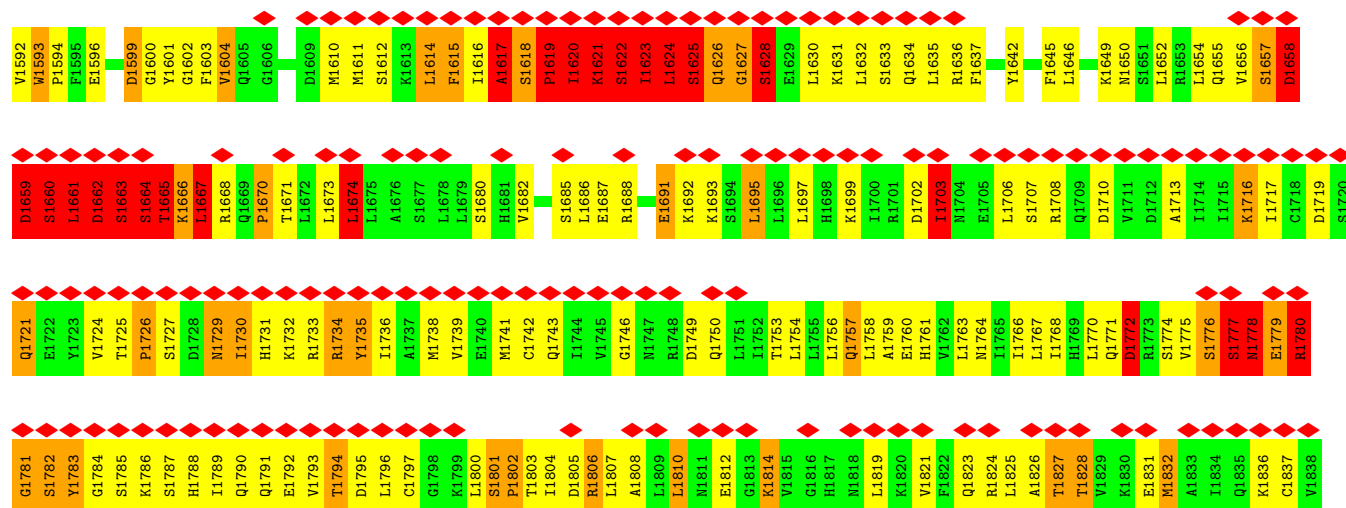




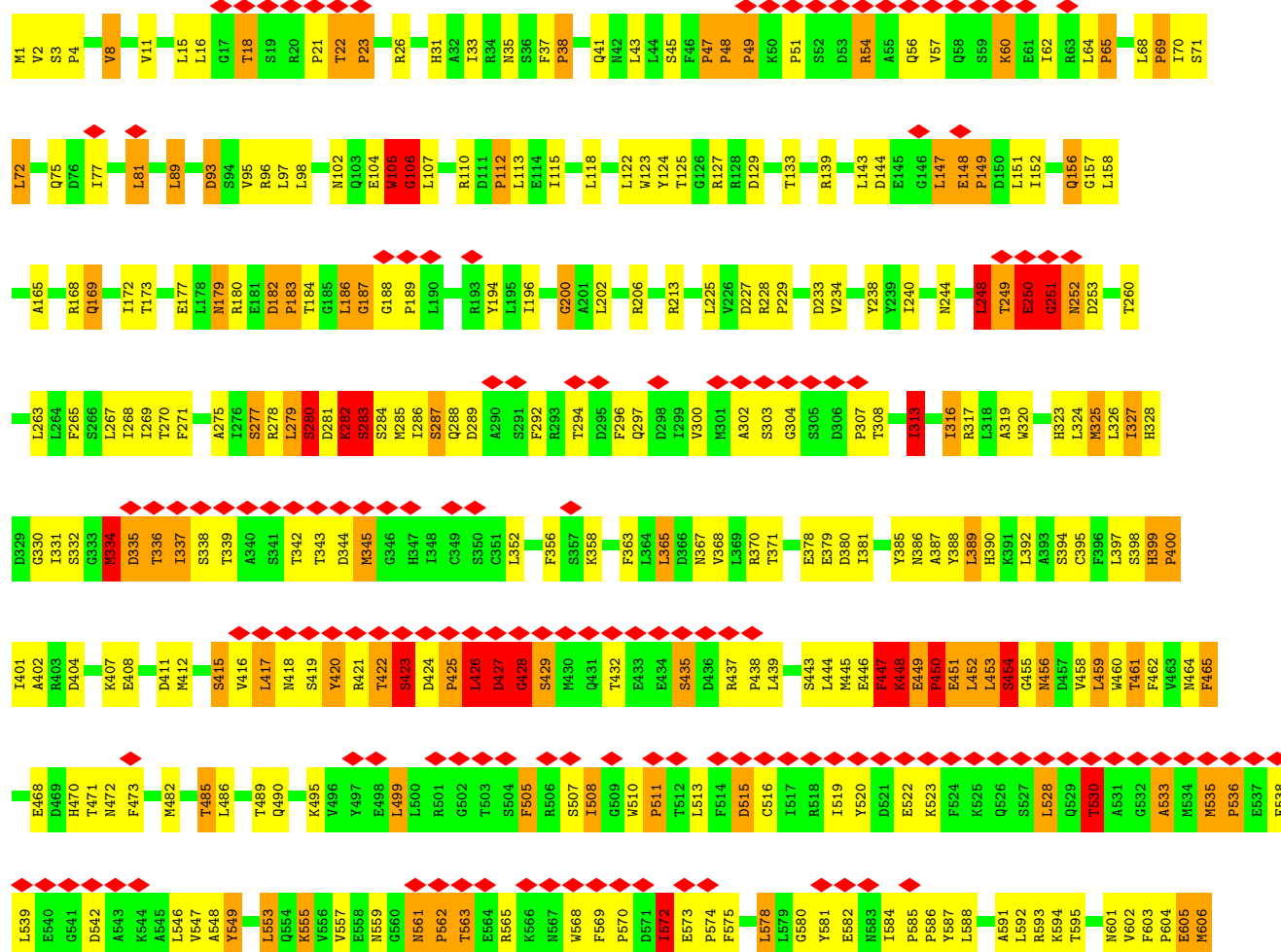
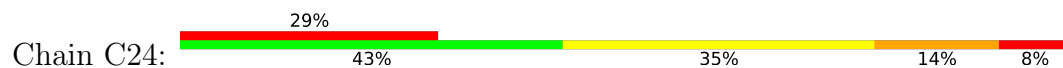
• Molecule 10: Nuclear pore complex protein NUP205

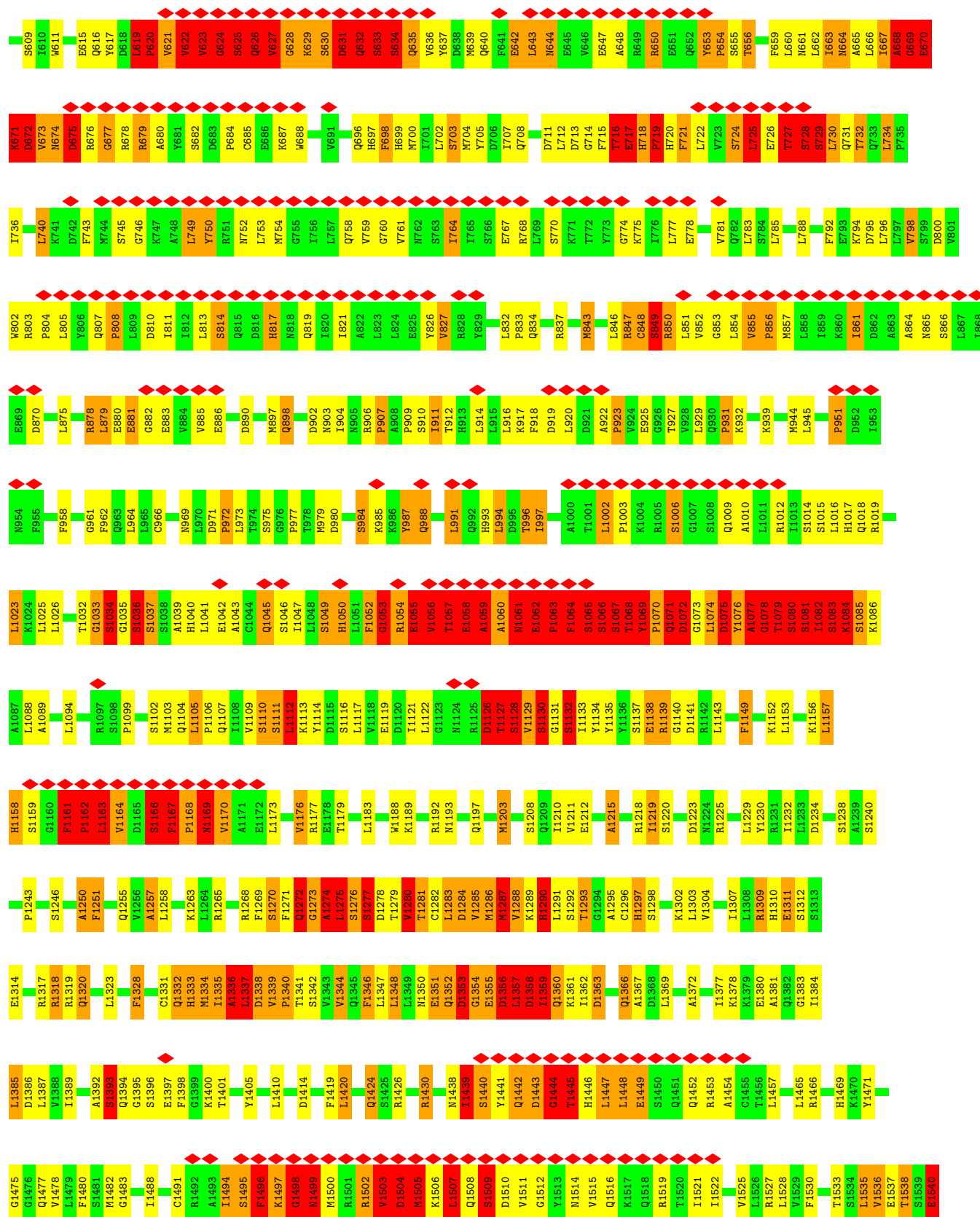


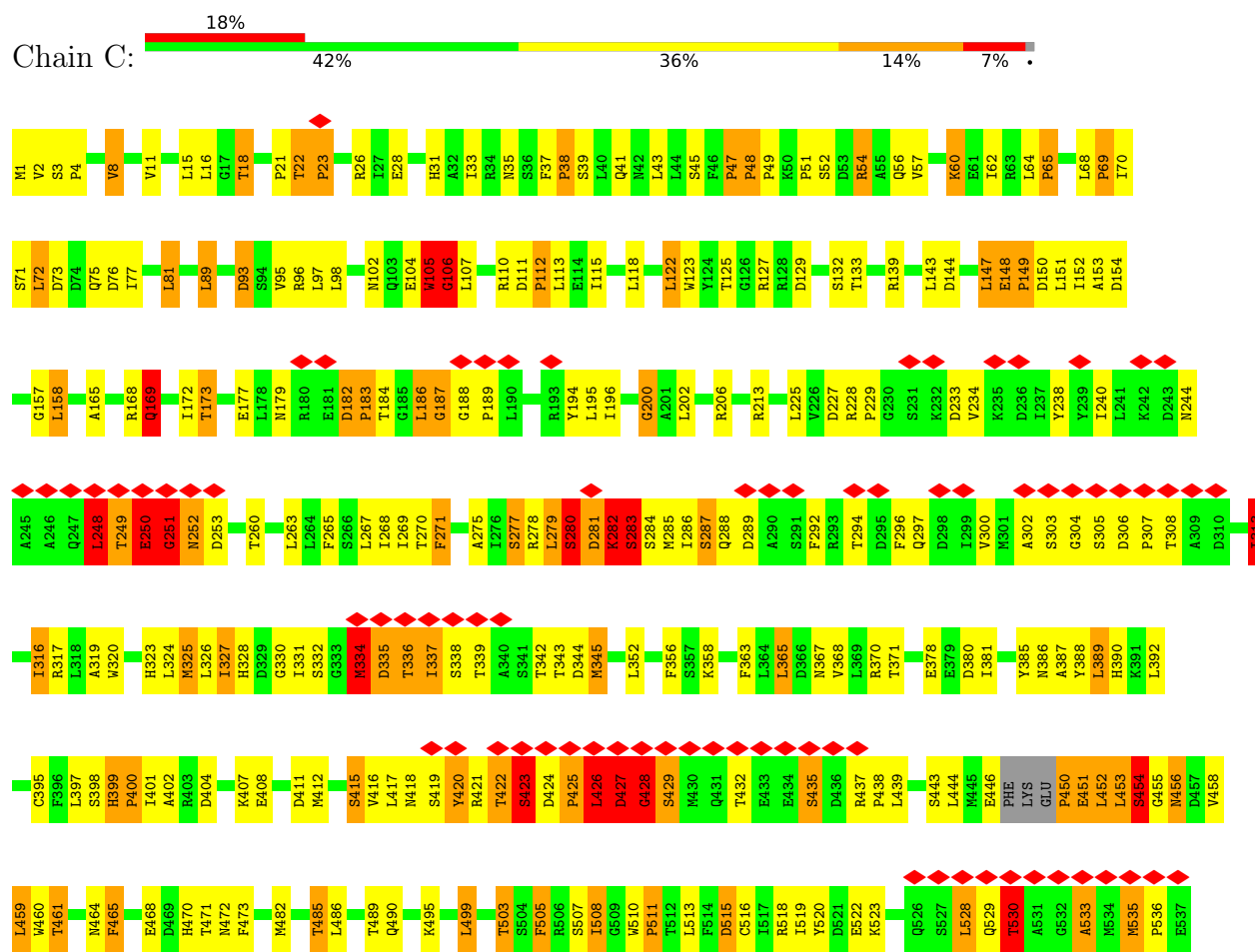
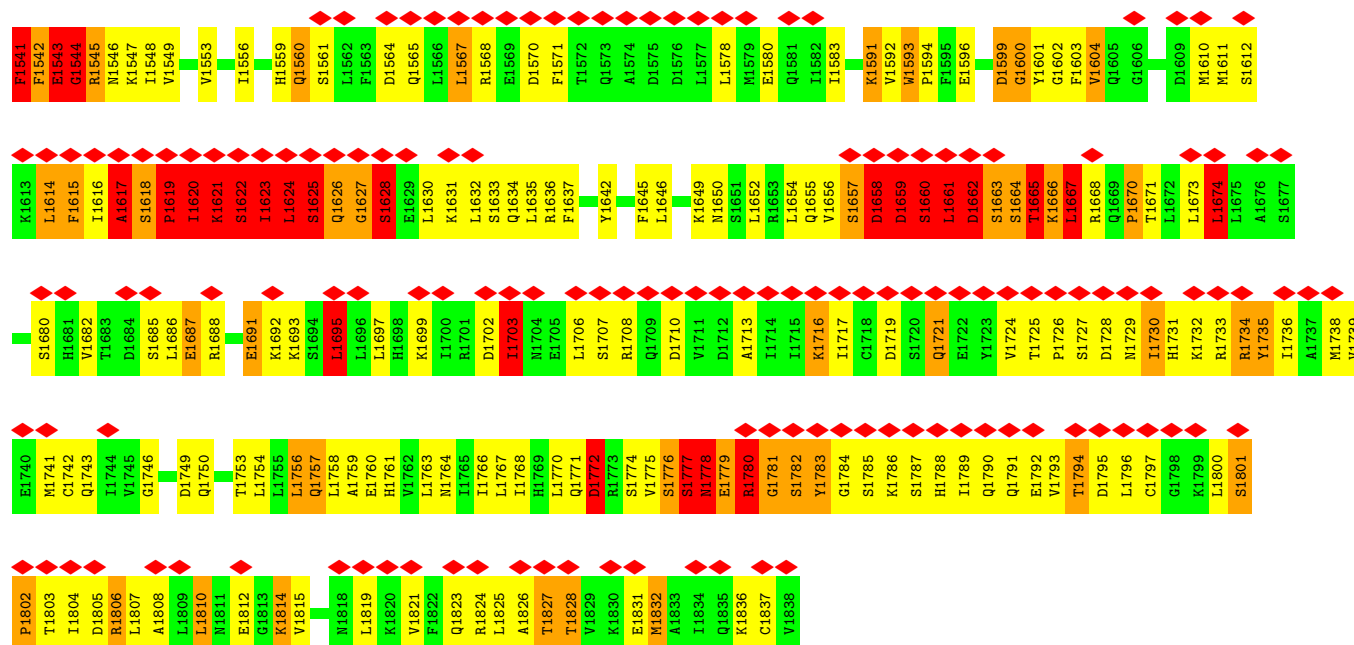


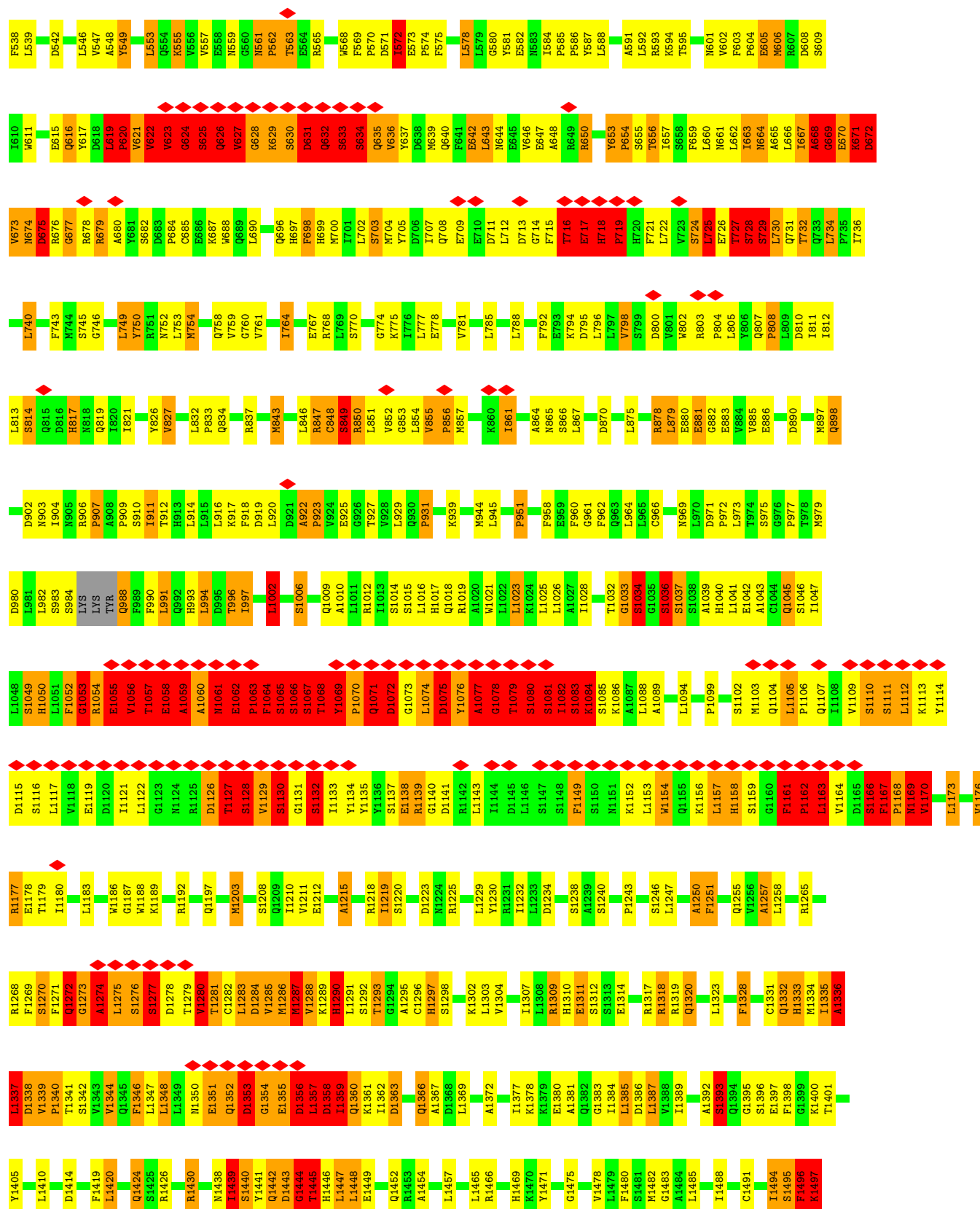


• Molecule 10: Nuclear pore complex protein NUP205

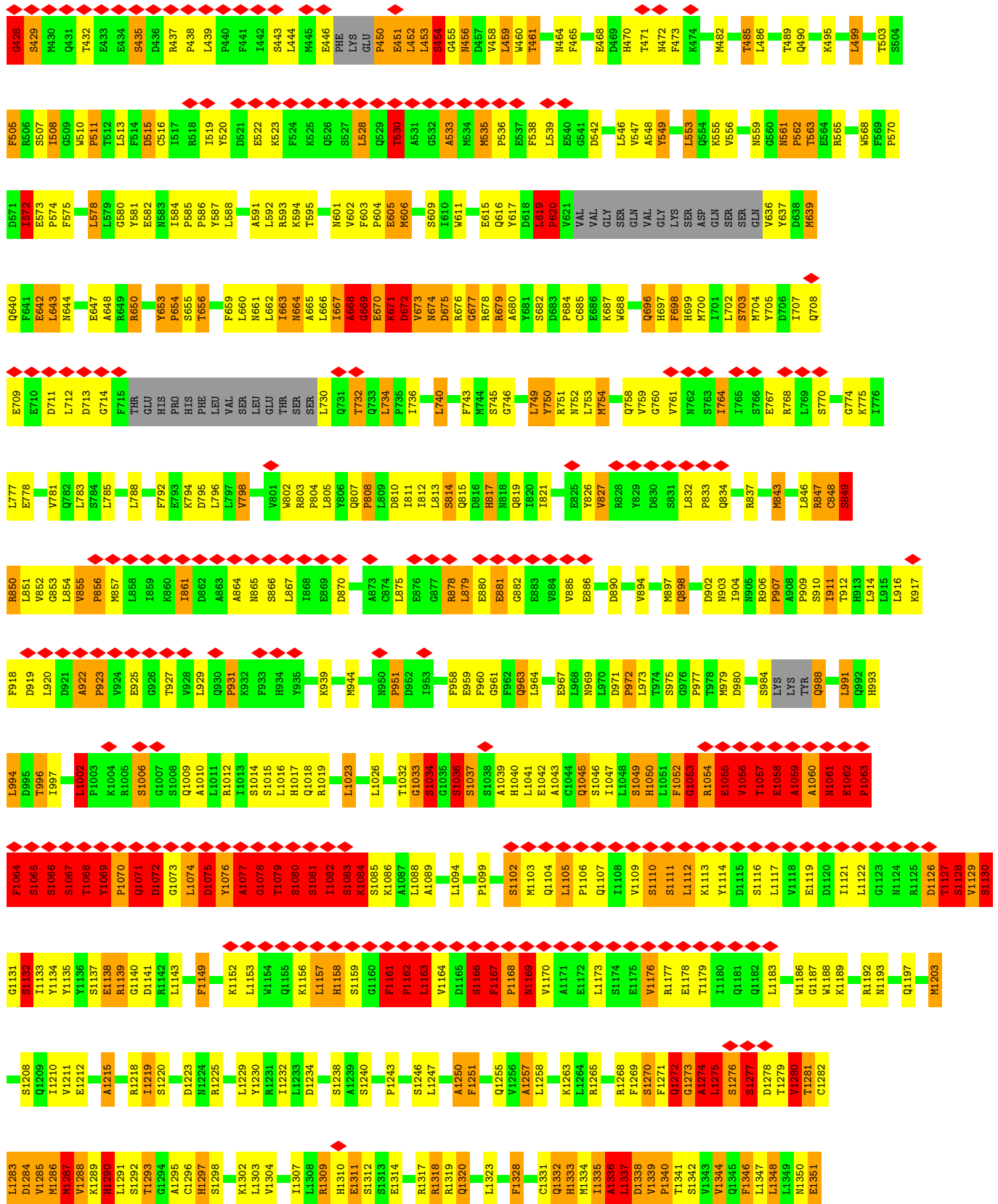


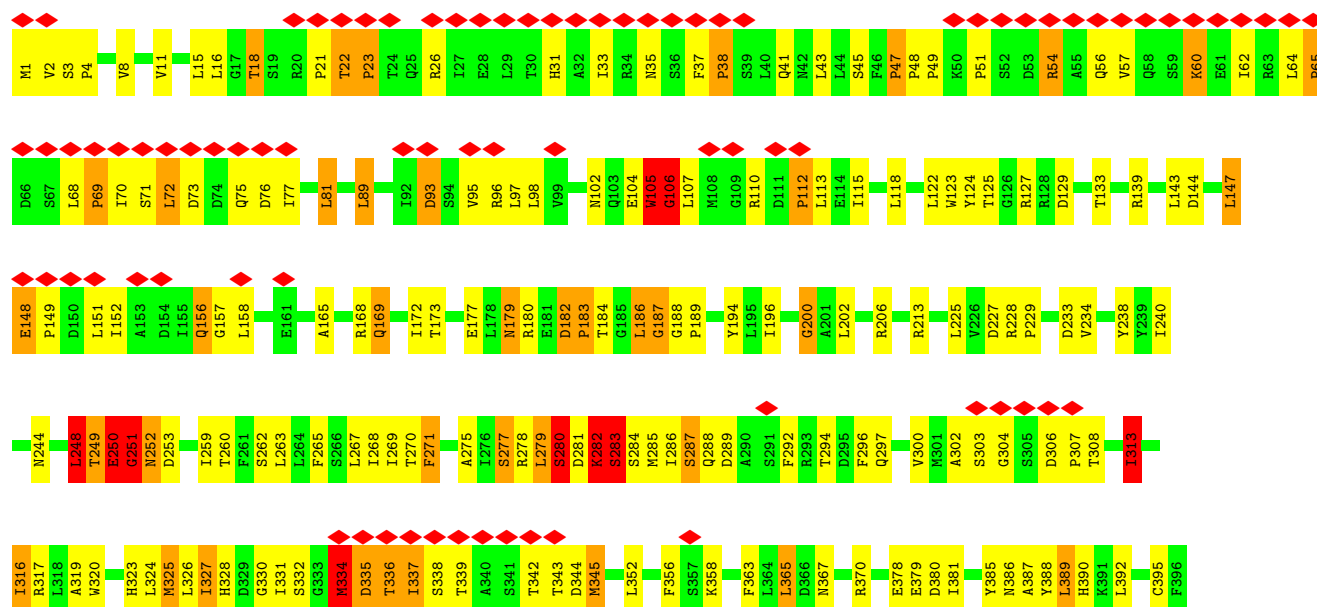
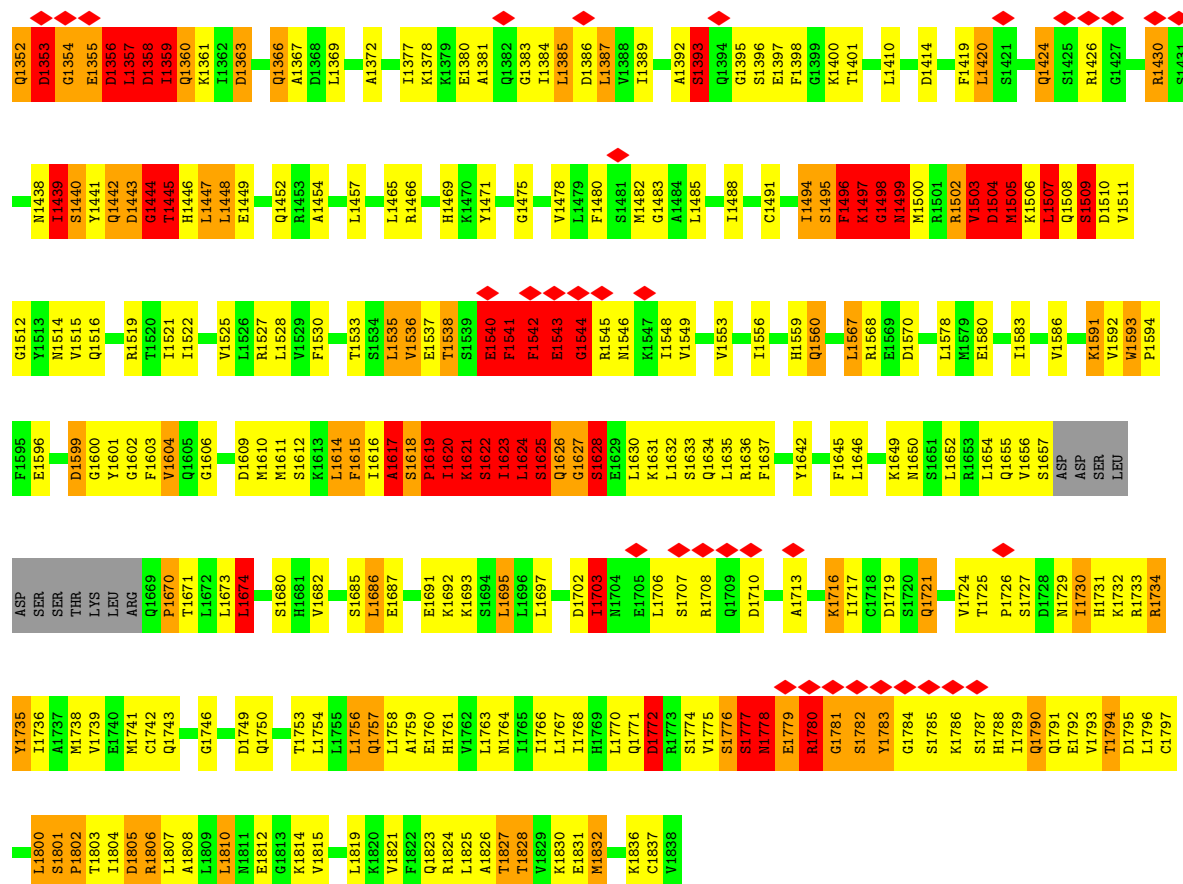




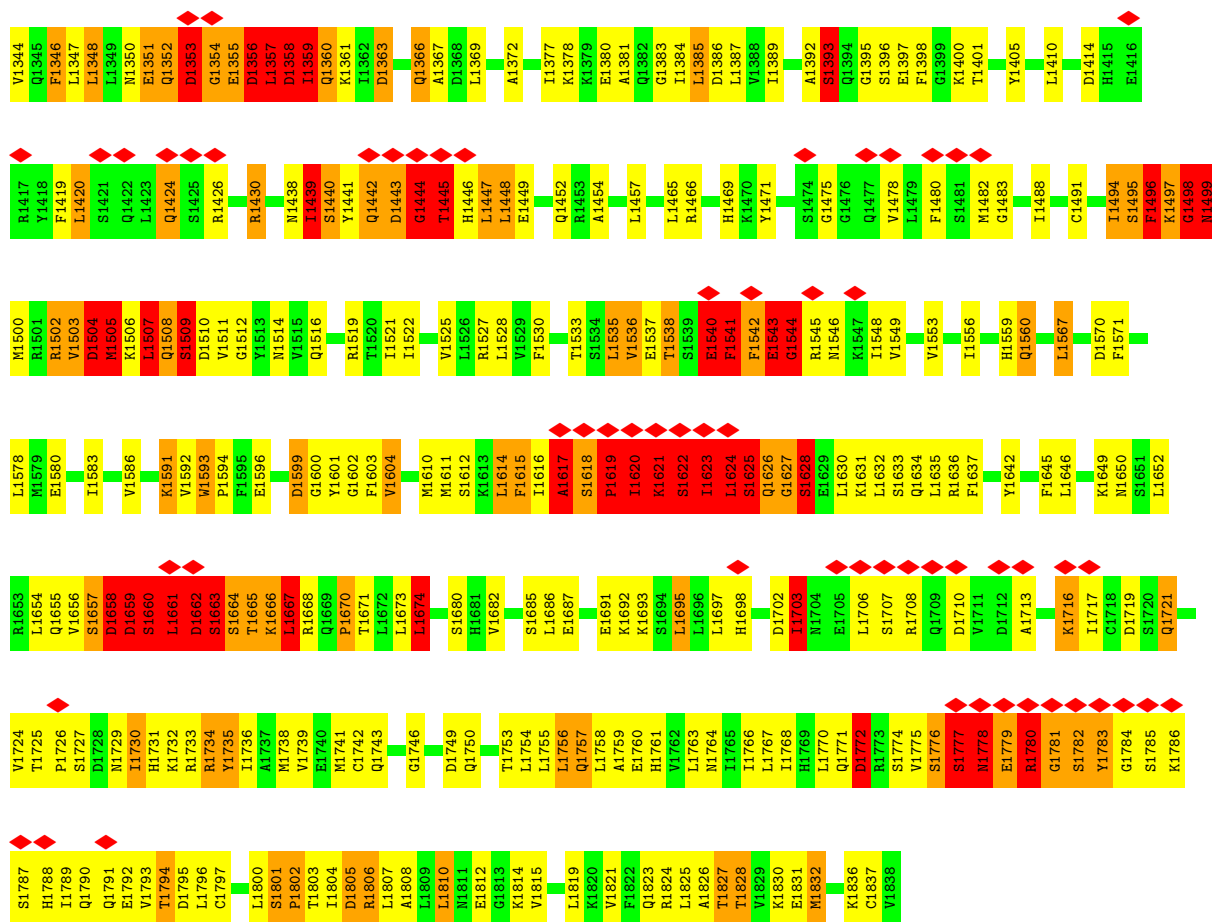




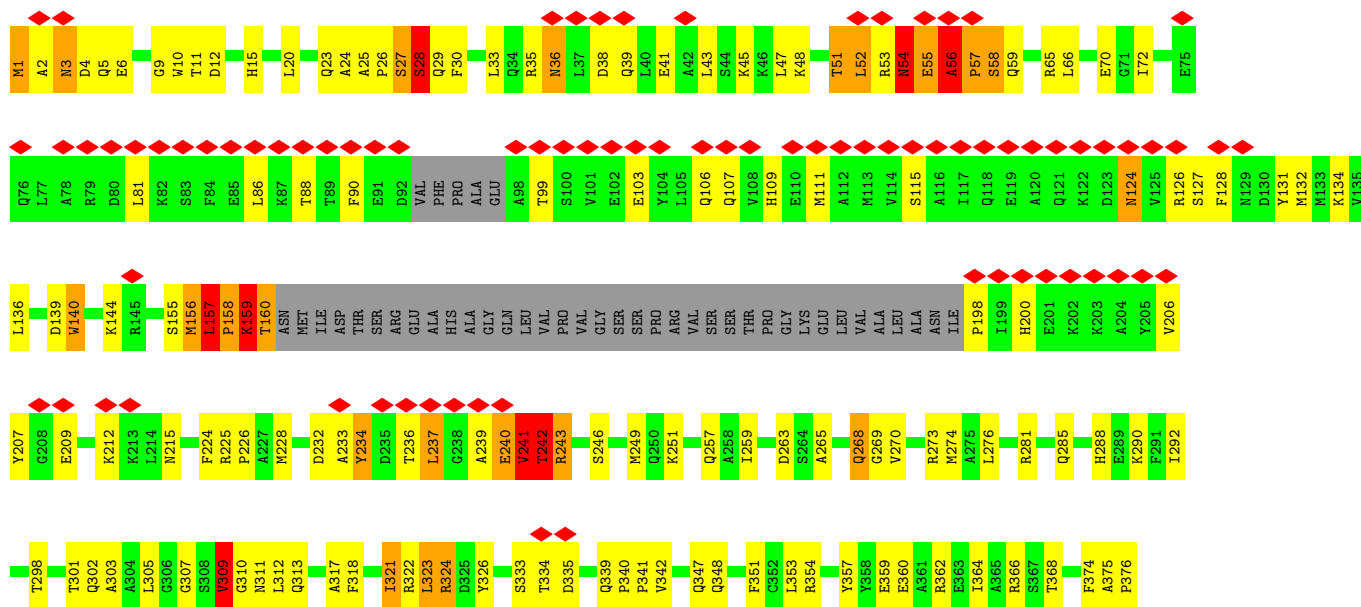


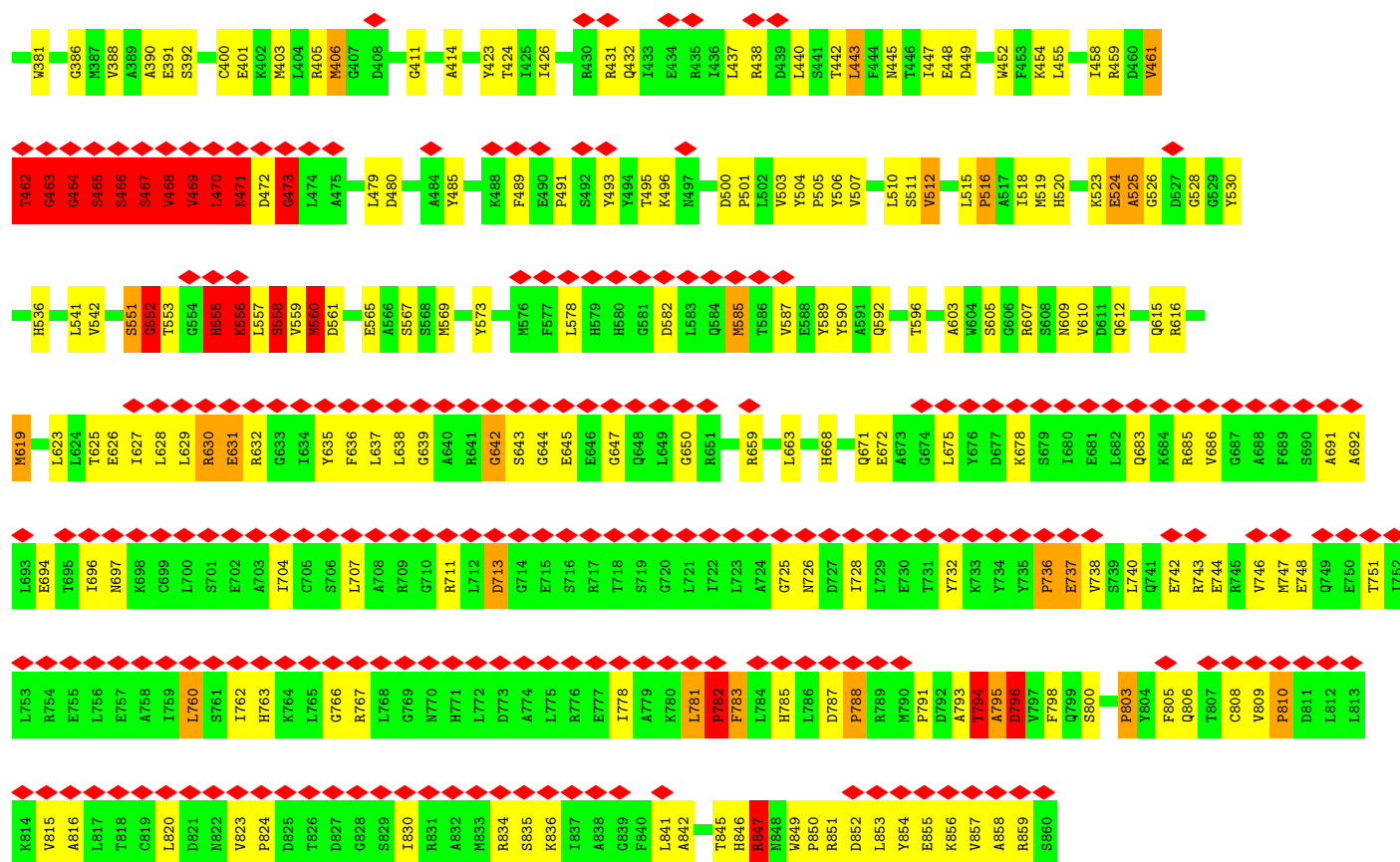




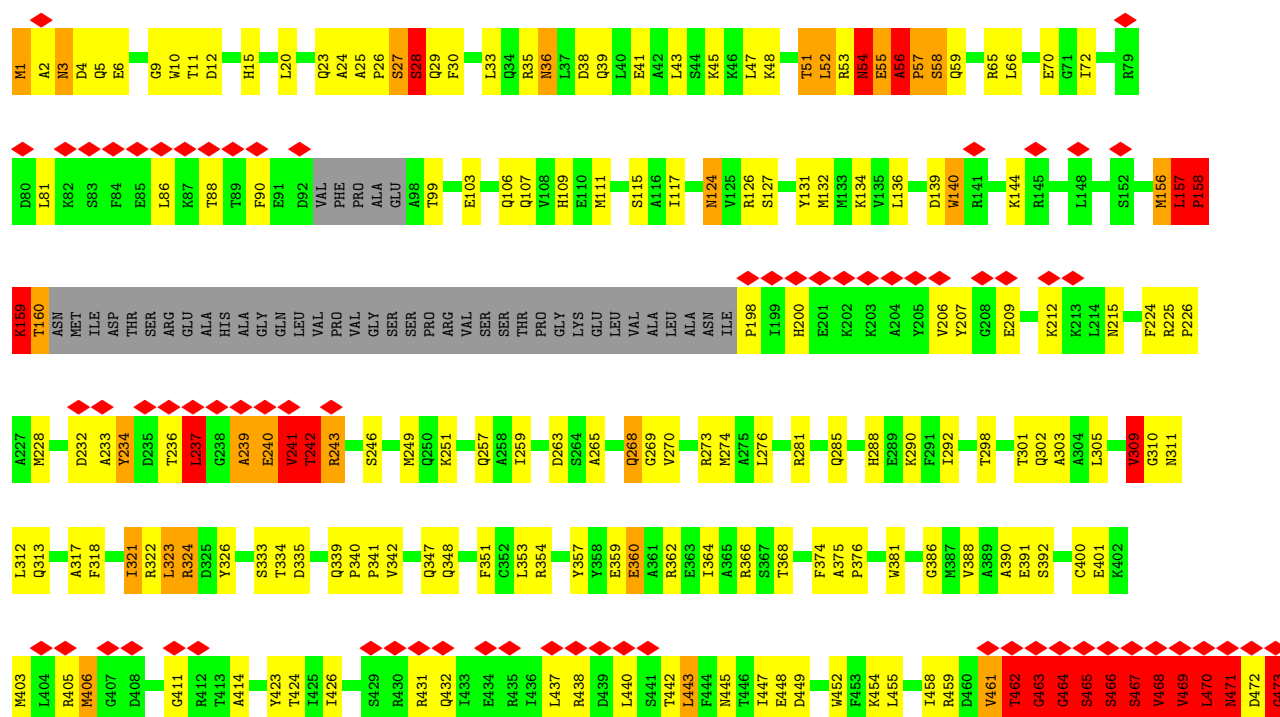


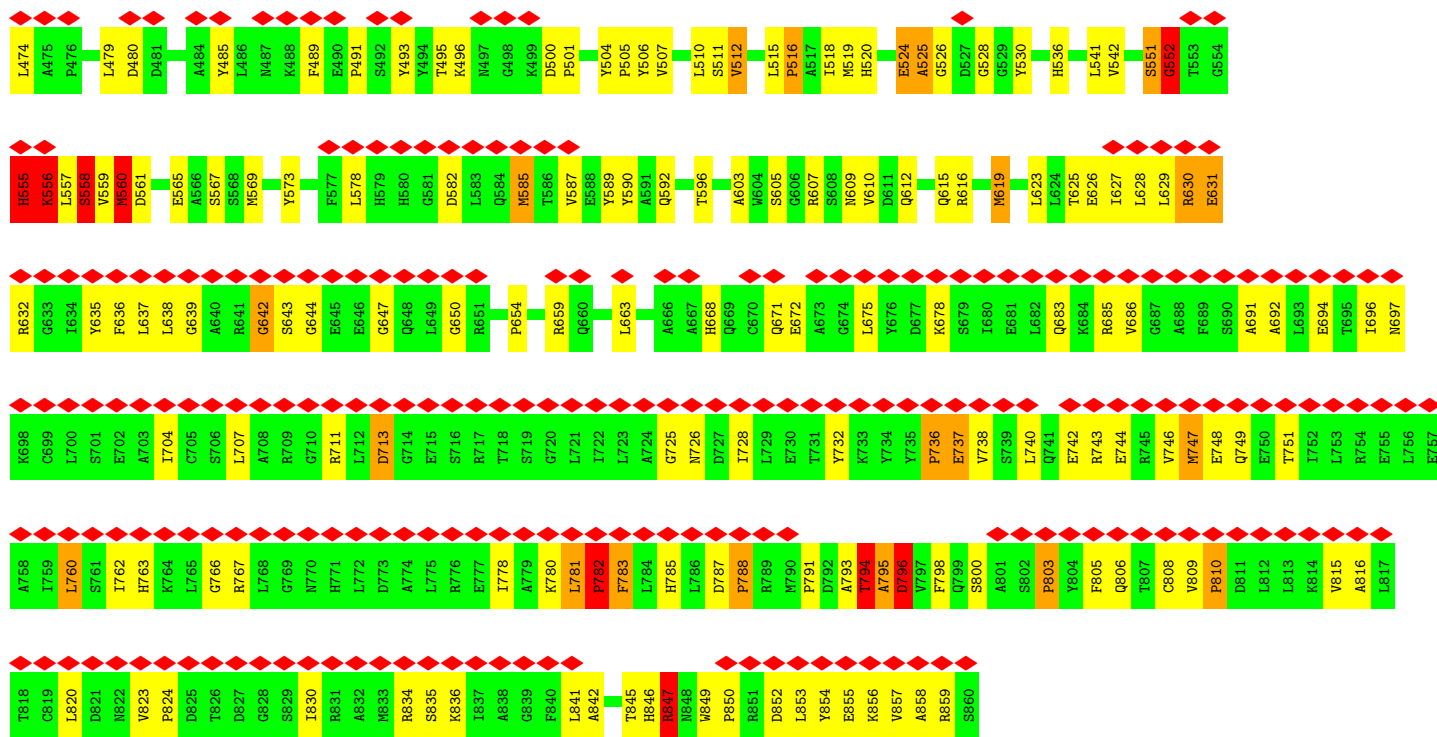
• Molecule 11: Nuclear pore complex protein NUP93A



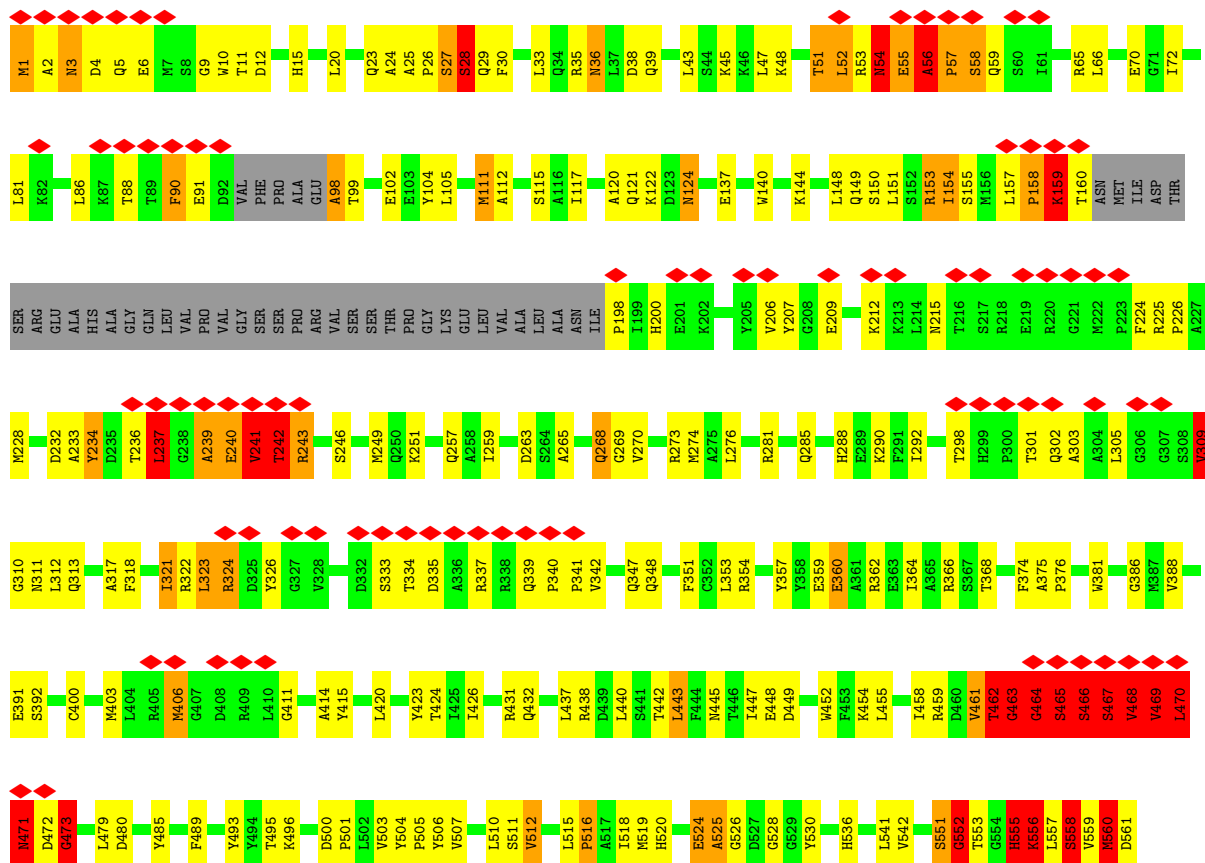


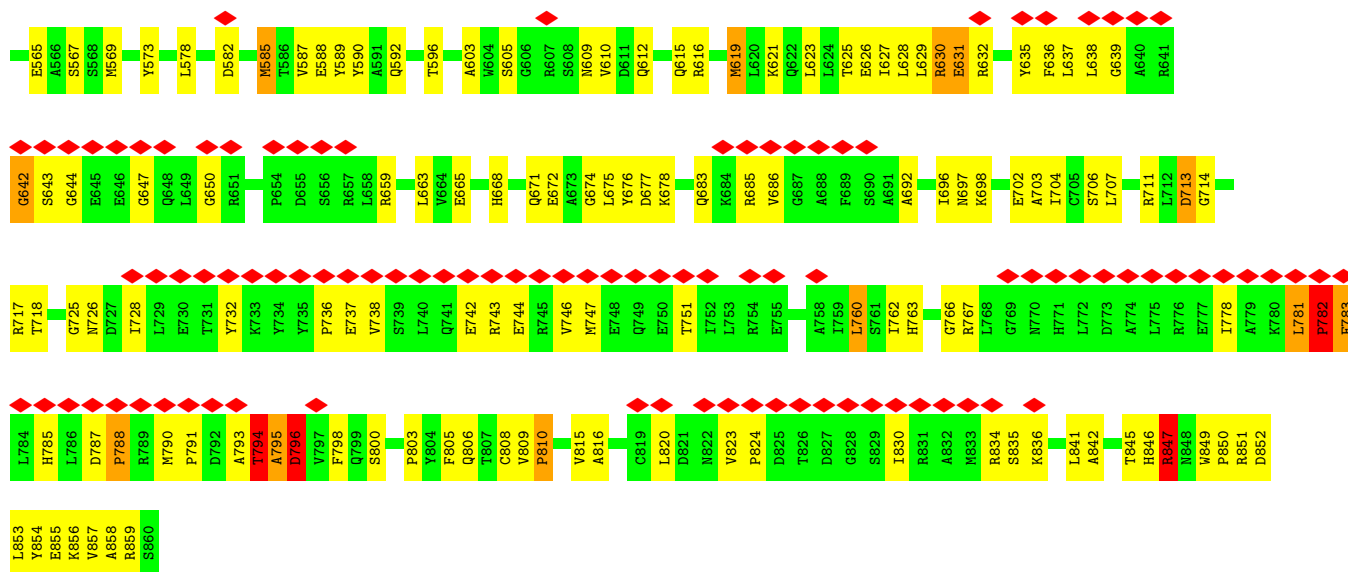
### • Molecule 11: Nuclear pore complex protein NUP93A



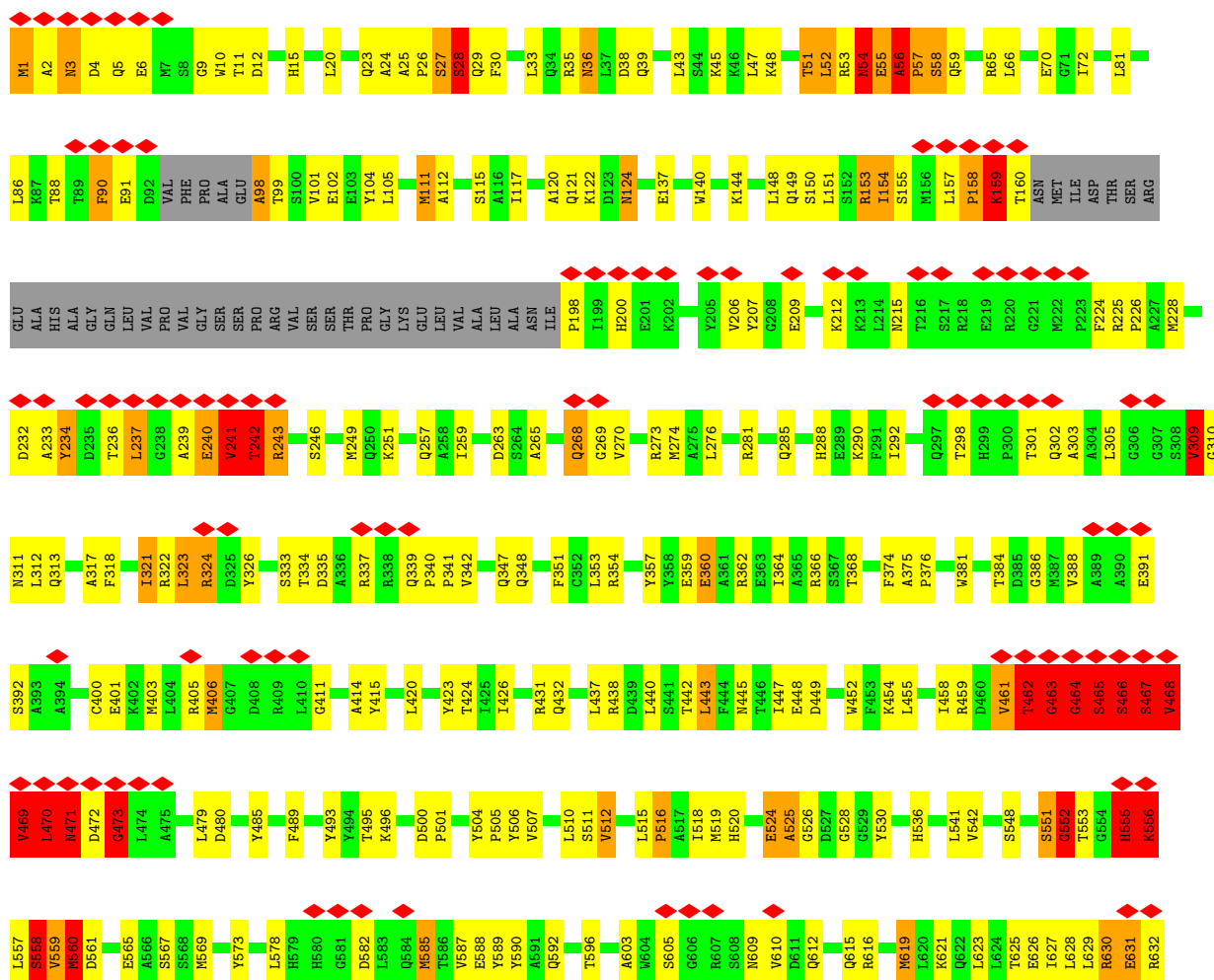


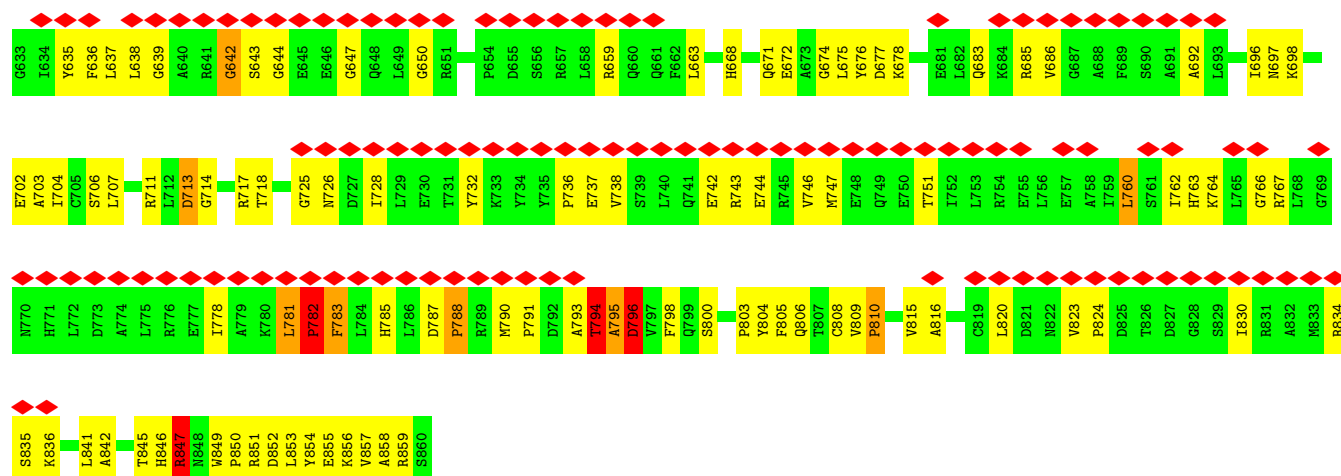
• Molecule 11: Nuclear pore complex protein NUP93A



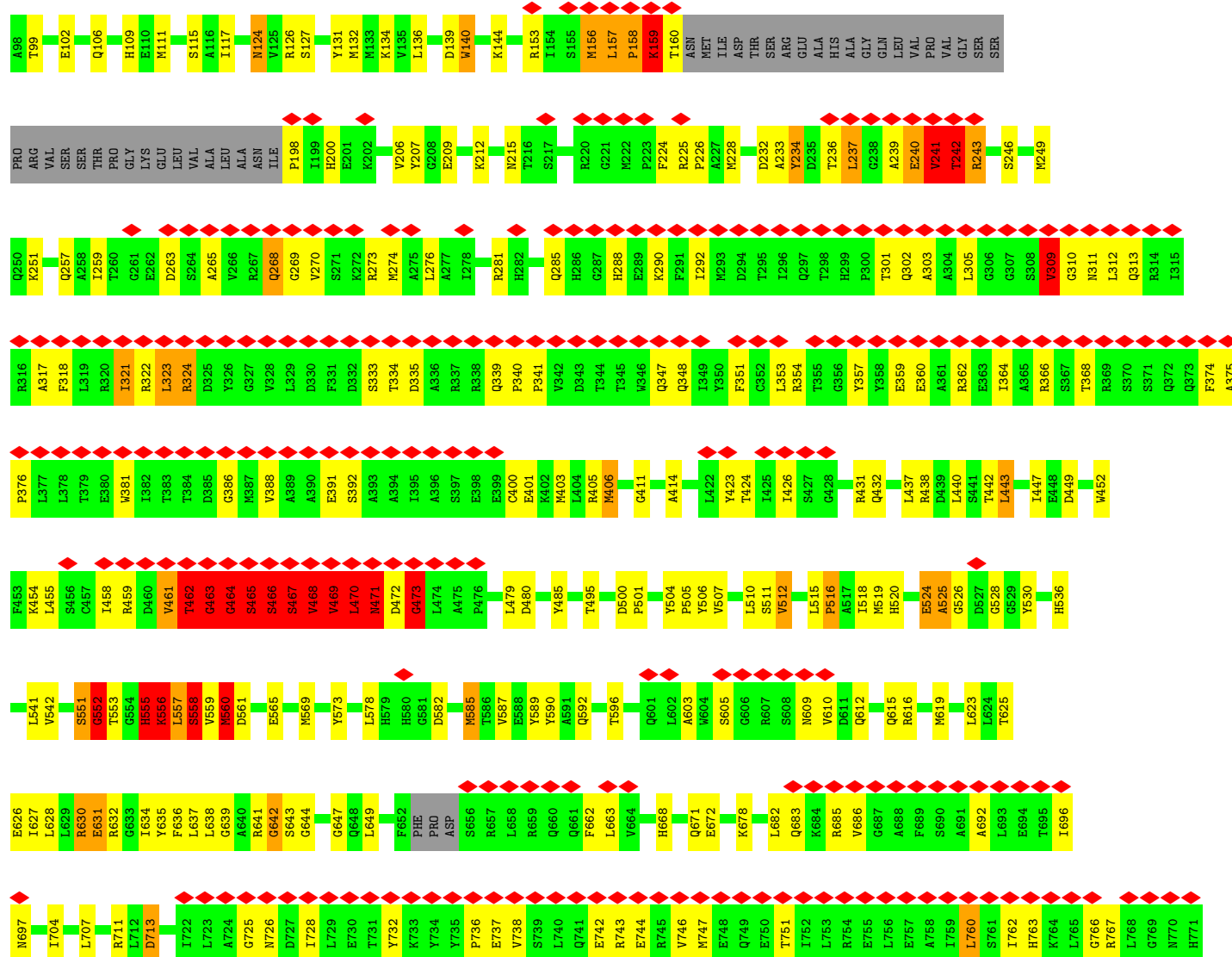


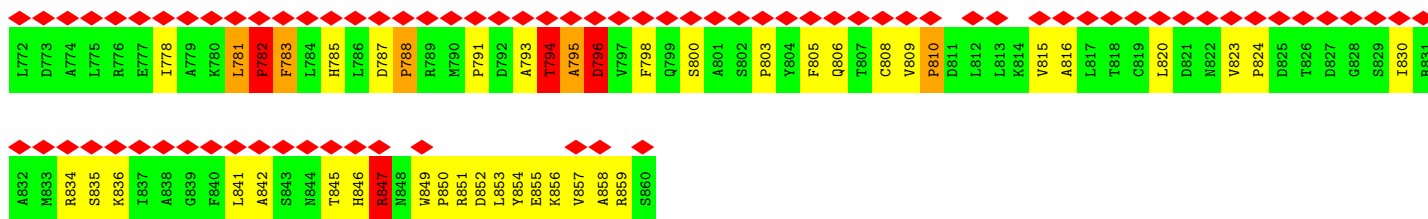
• Molecule 11: Nuclear pore complex protein NUP93A





• Molecule 12: Nuclear pore complex protein NUP93A





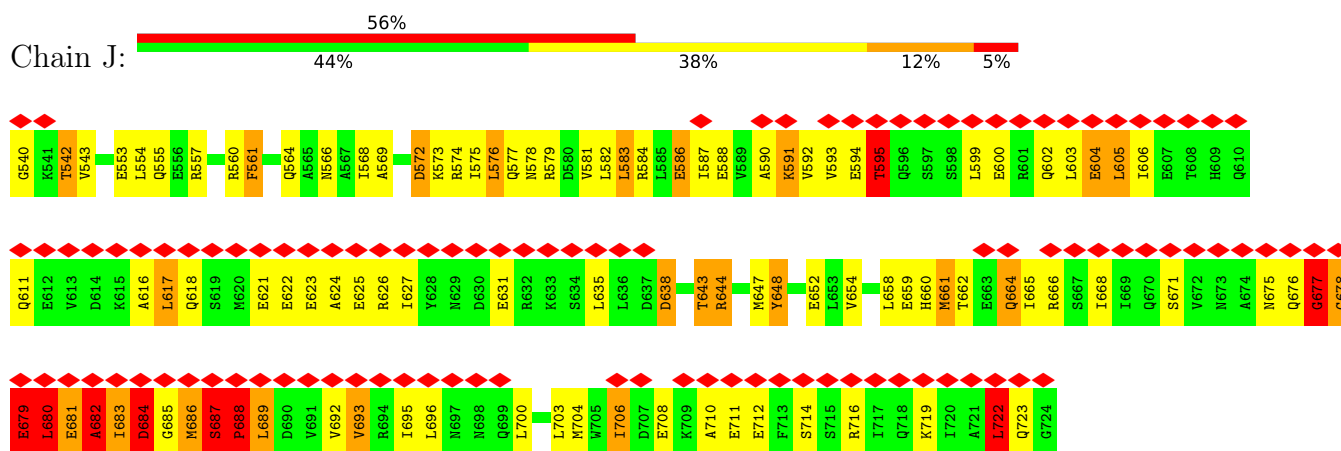
• Molecule 12: Nuclear pore complex protein NUP93A



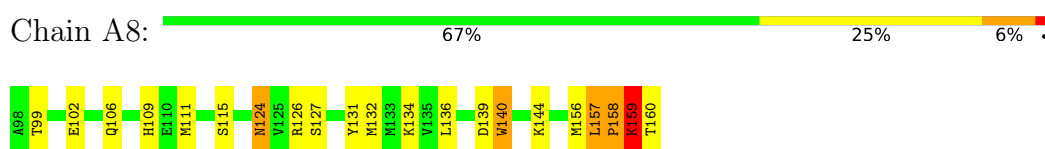
• Molecule 13: Nuclear pore complex protein NUP214



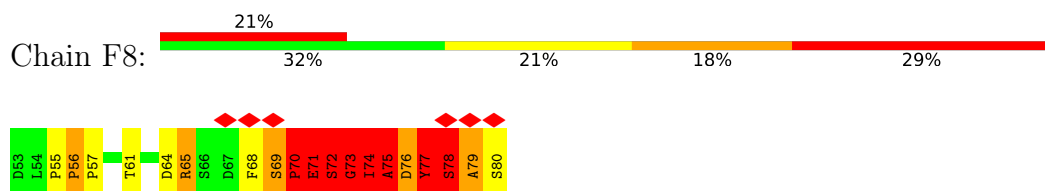
- Molecule 15: Nuclear pore complex protein NUP62



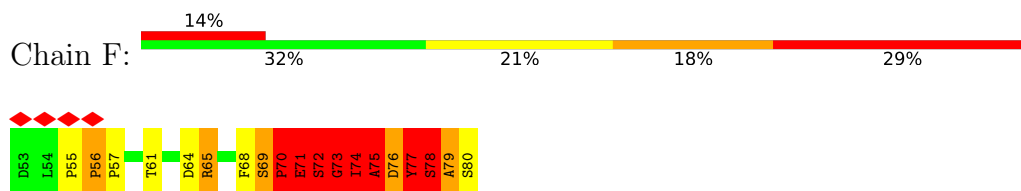
- Molecule 16: Nuclear pore complex protein NUP93A



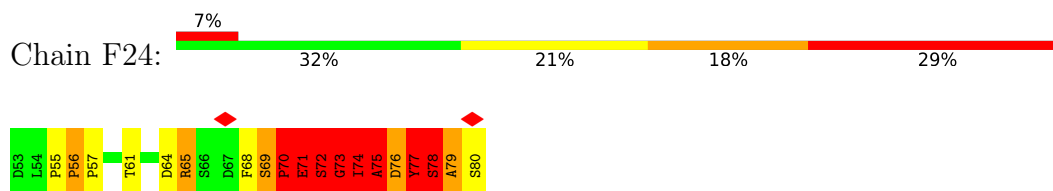
- Molecule 17: Nuclear pore complex protein NUP35



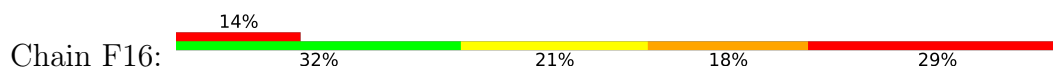
- Molecule 17: Nuclear pore complex protein NUP35

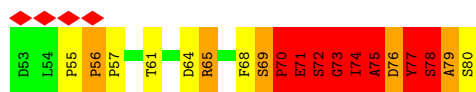


- Molecule 17: Nuclear pore complex protein NUP35

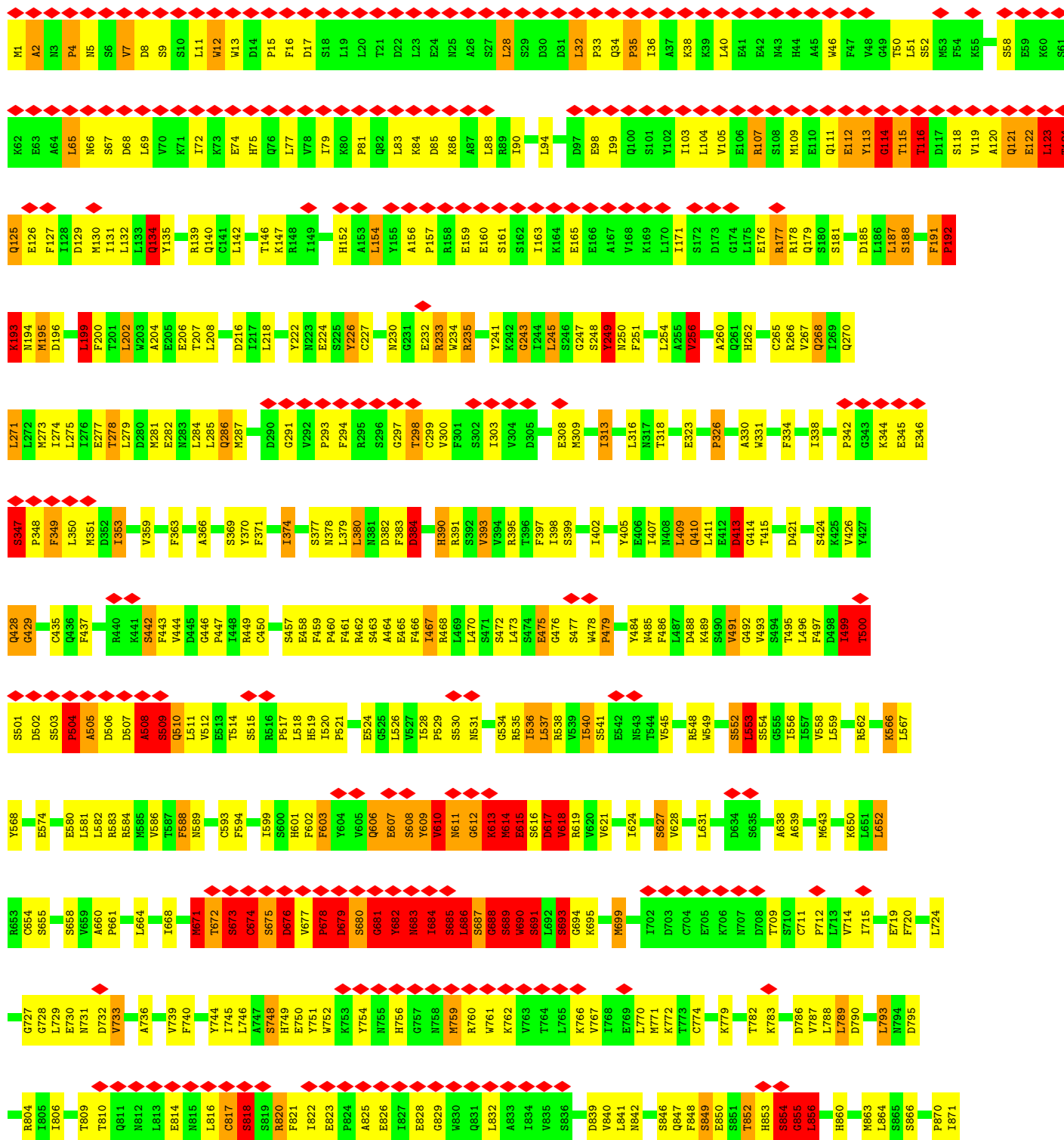


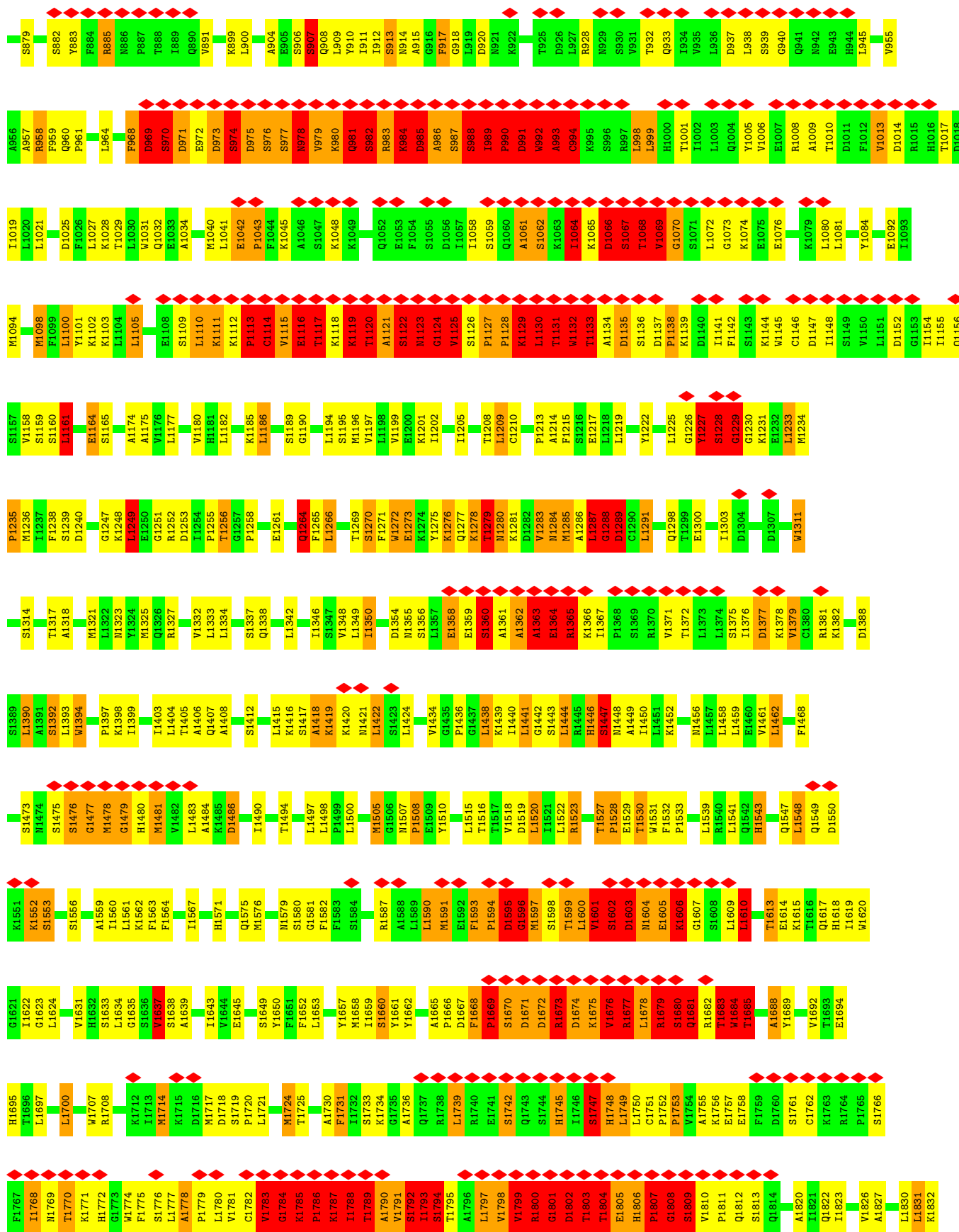
- Molecule 17: Nuclear pore complex protein NUP35

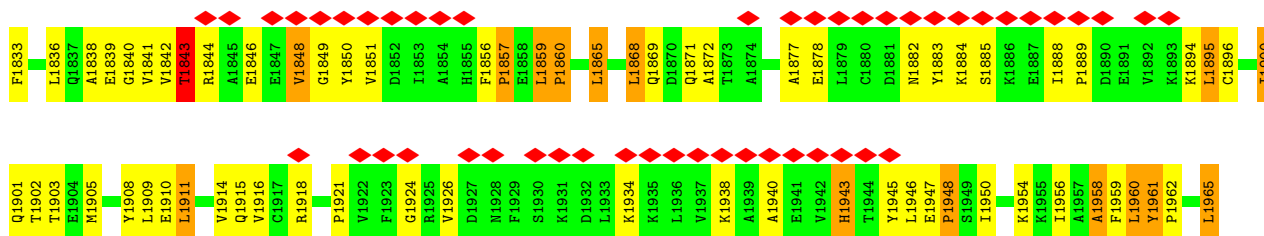




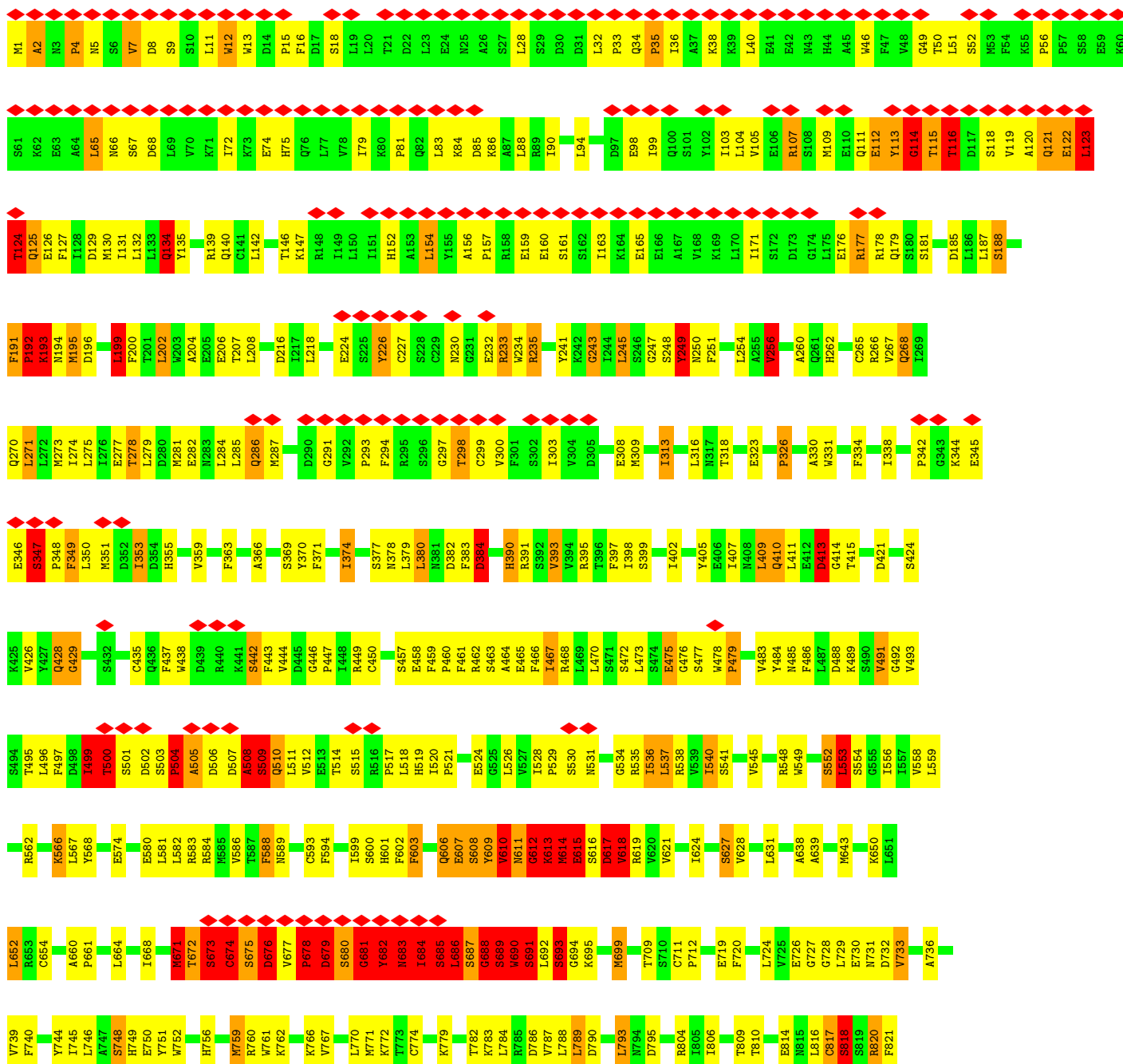
• Molecule 18: Nucleoporin (DUF3414)



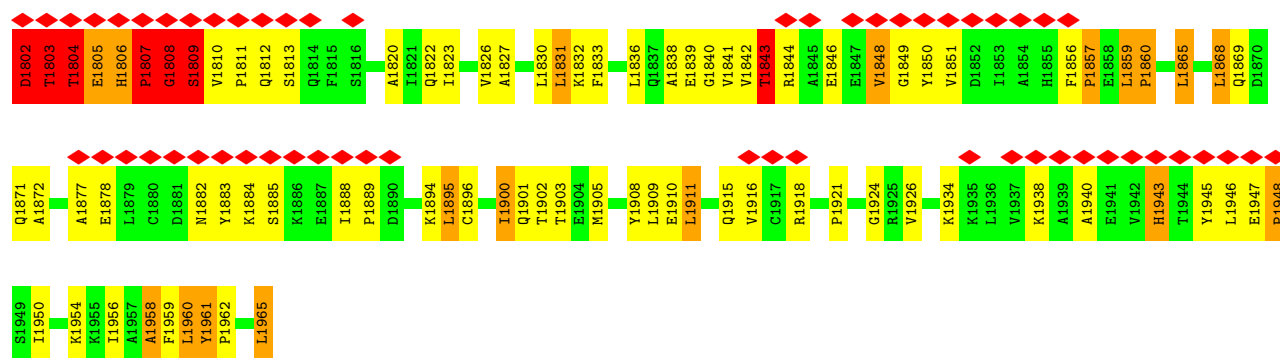




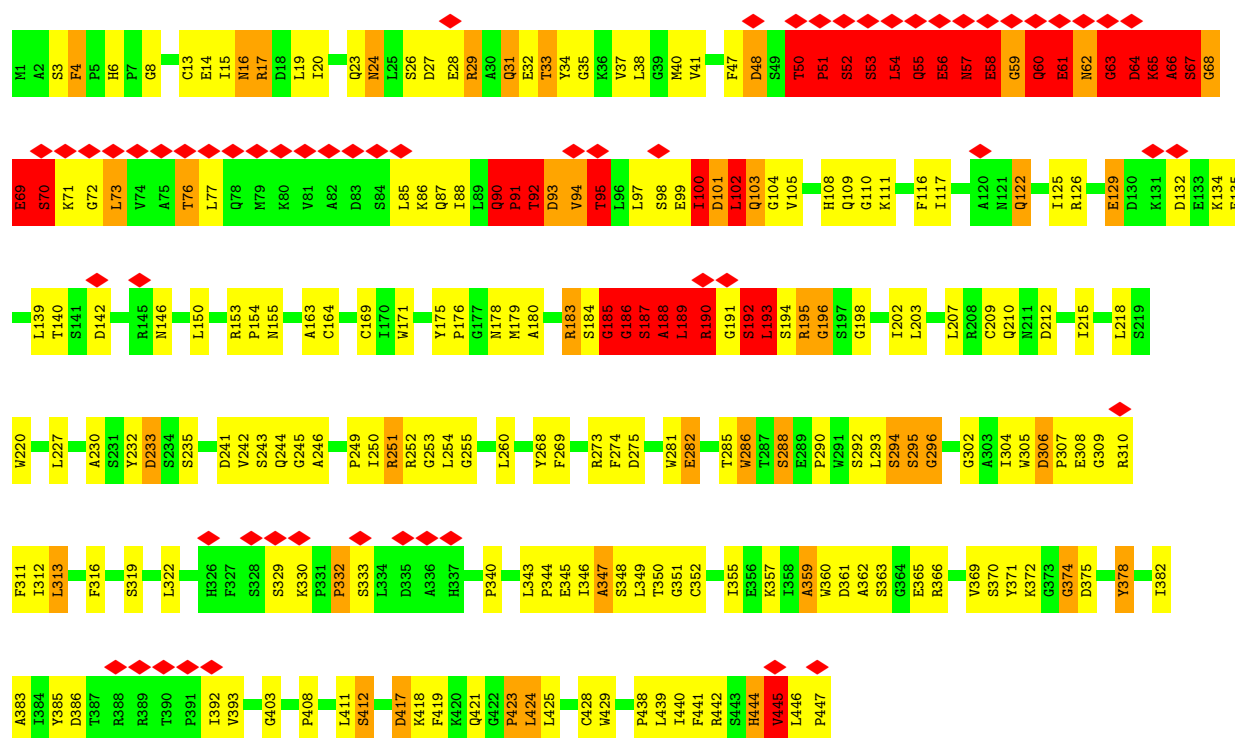
• Molecule 18: Nucleoporin (DUF3414)



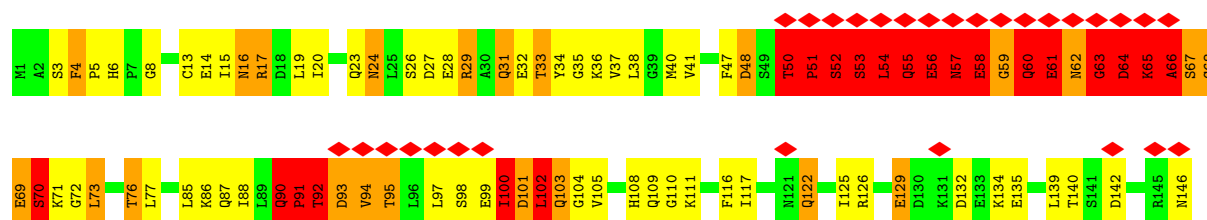


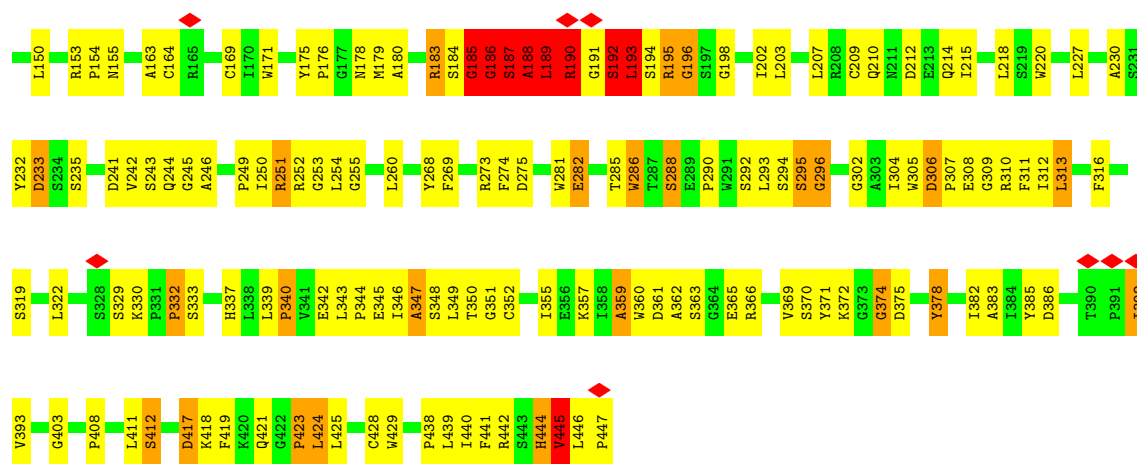


### • Molecule 19: Aladin

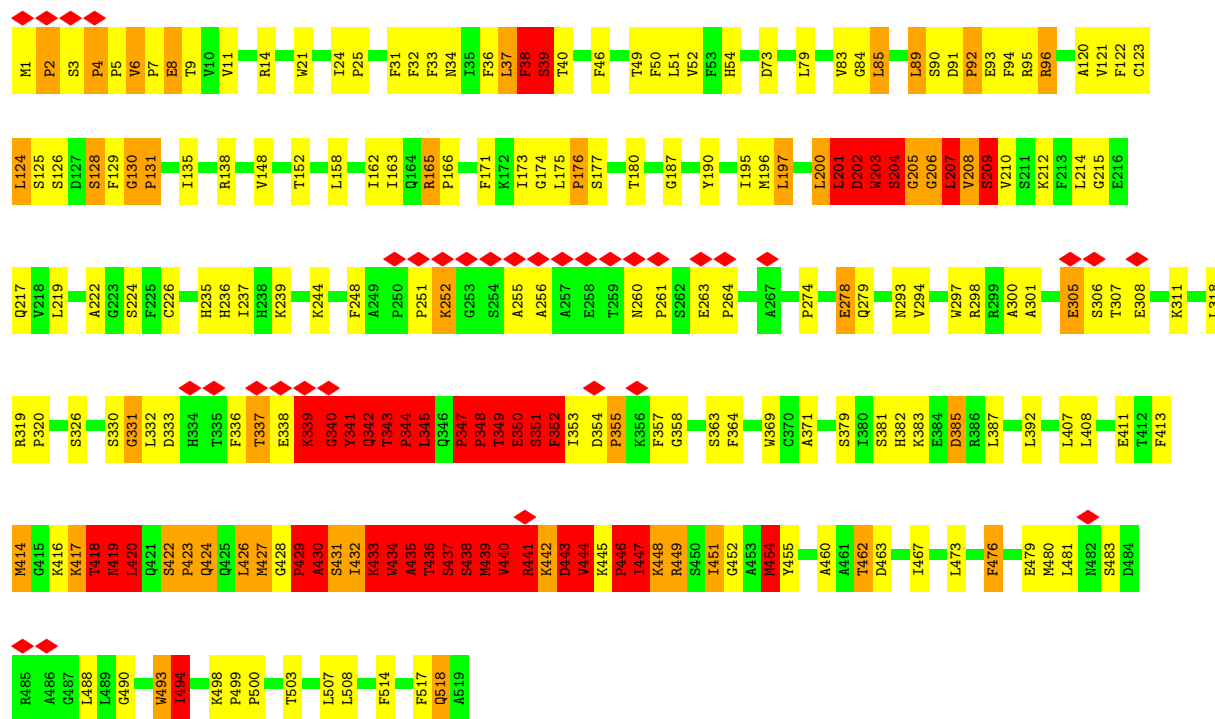


### • Molecule 19: Aladin

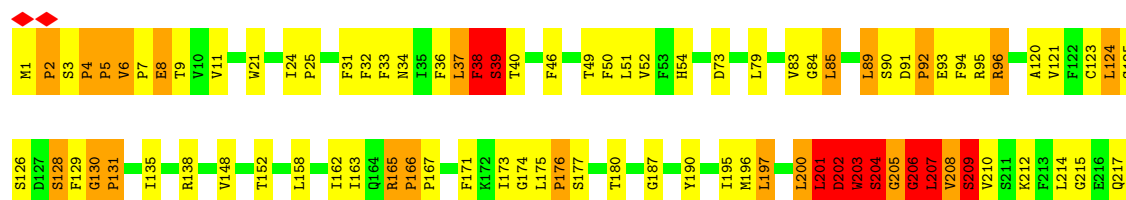


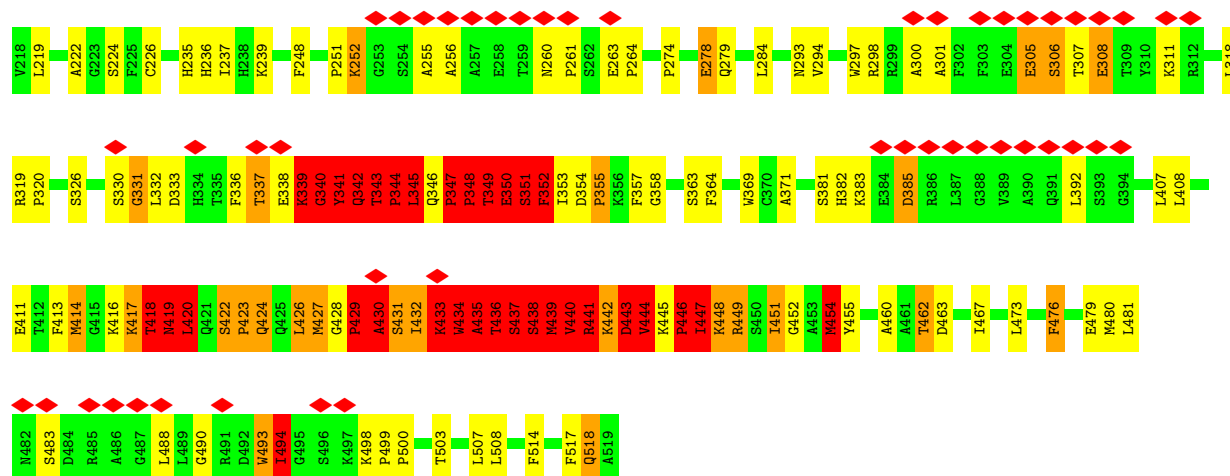


• Molecule 20: Nucleoporin protein Ndc1-Nup protein

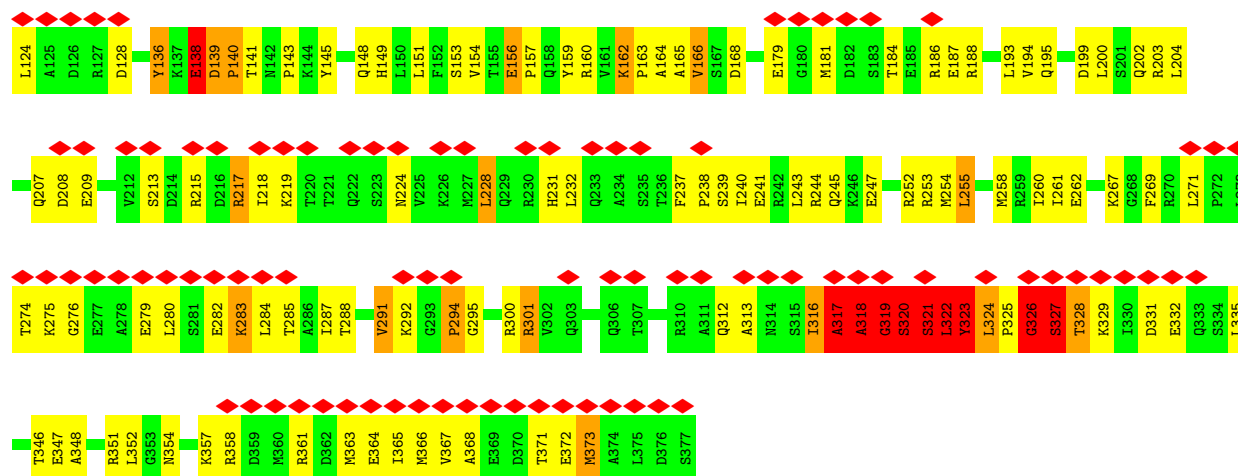


• Molecule 20: Nucleoporin protein Ndc1-Nup protein

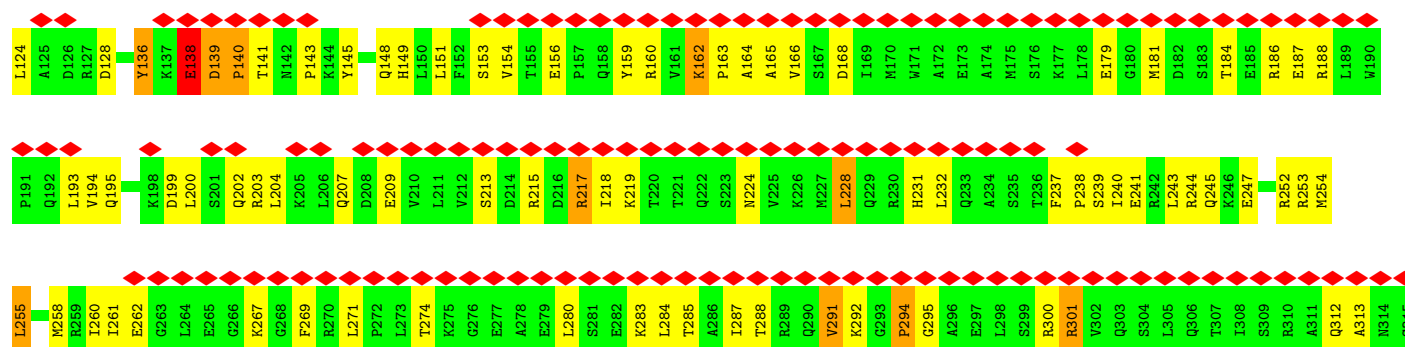


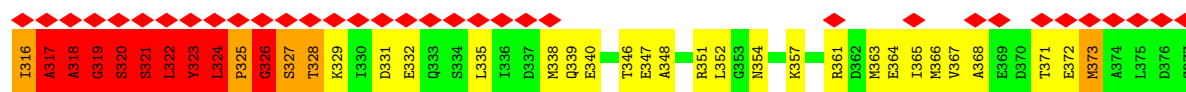


• Molecule 21: Nuclear pore complex protein NUP54

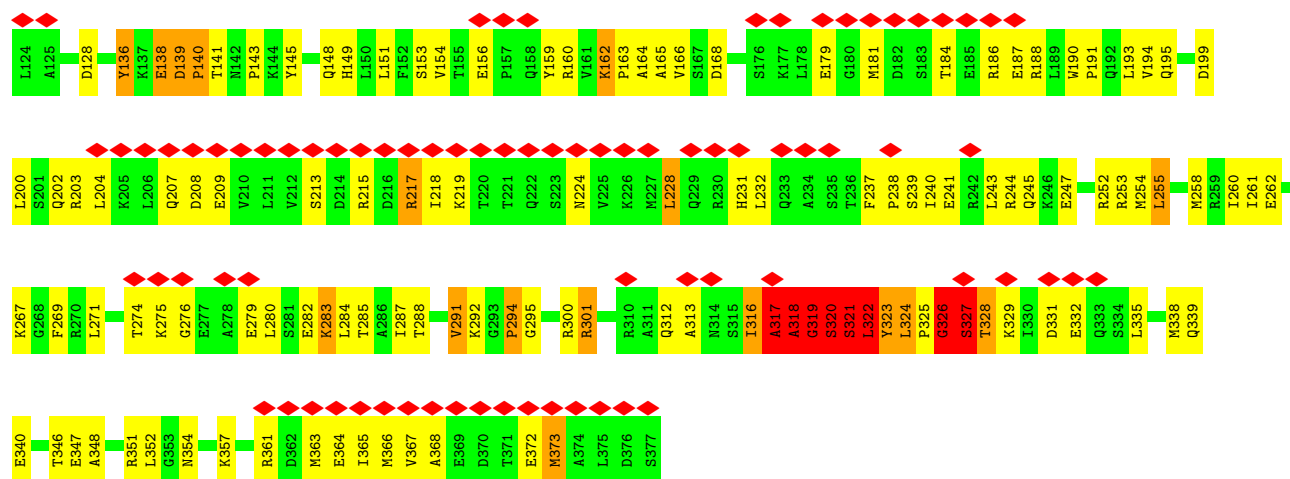


• Molecule 21: Nuclear pore complex protein NUP54

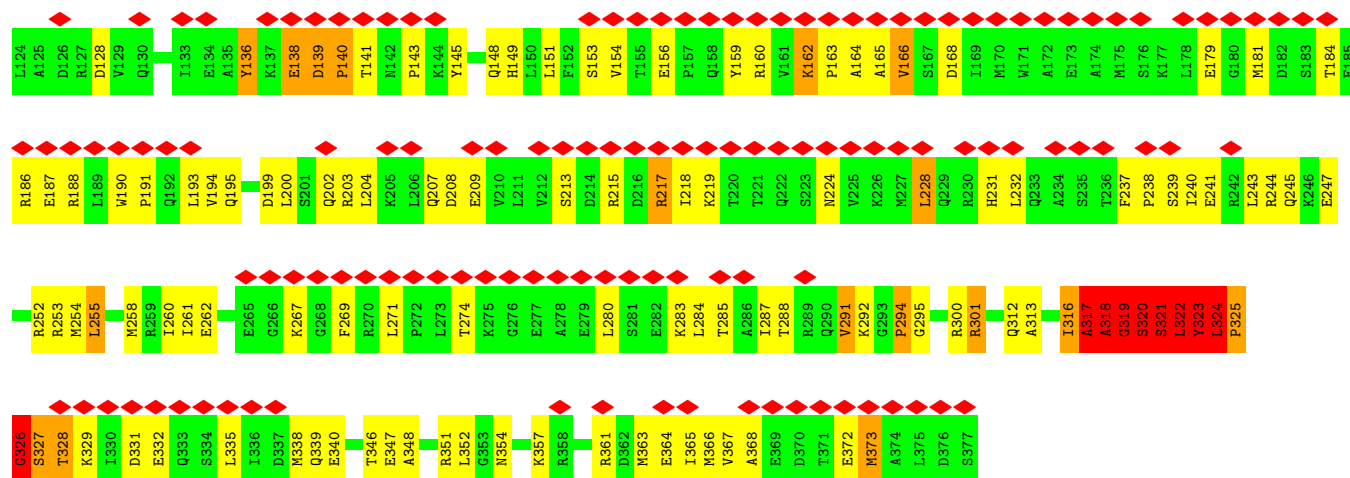




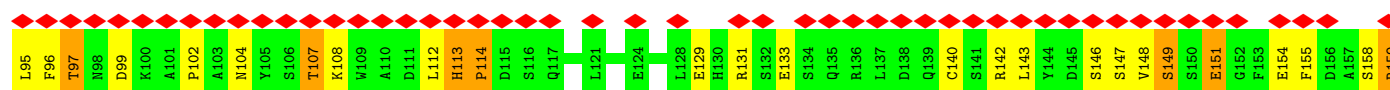
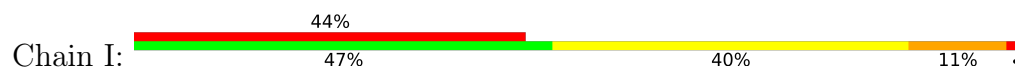
• Molecule 21: Nuclear pore complex protein NUP54

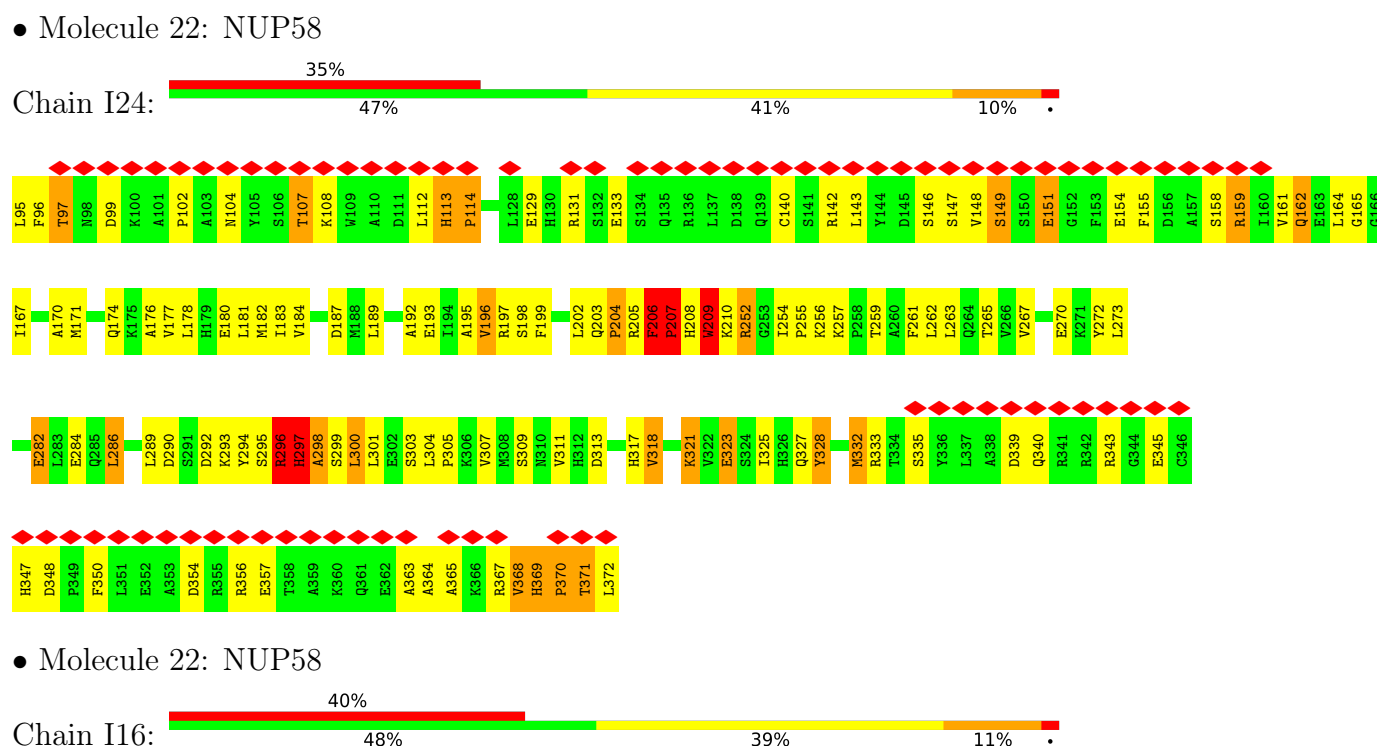
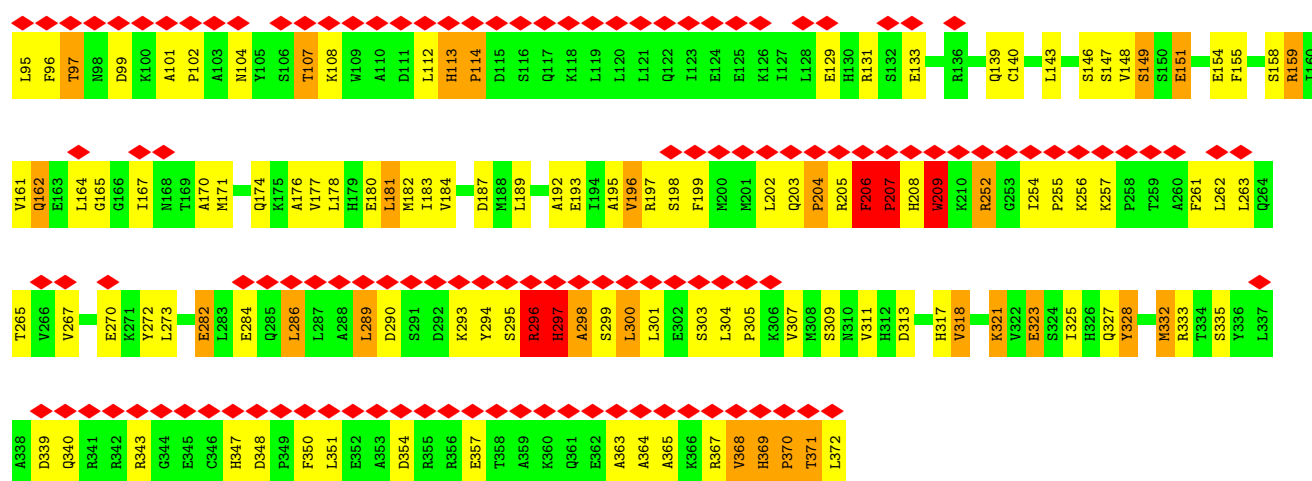
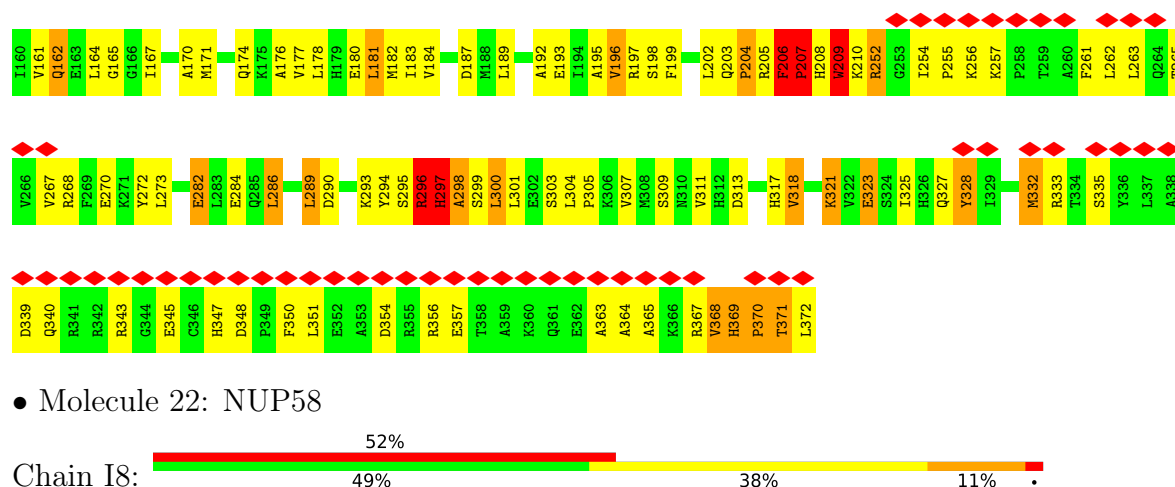


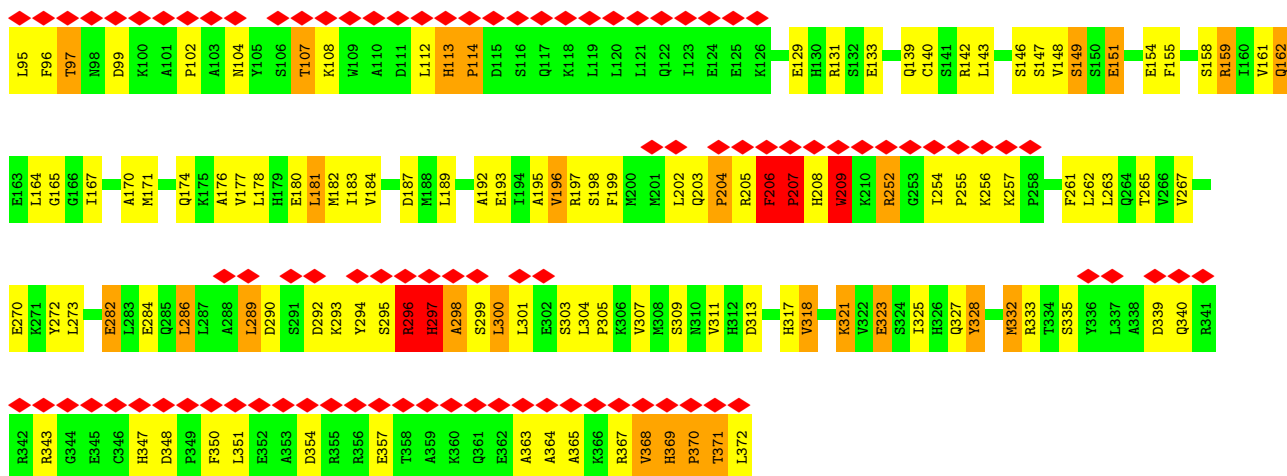
• Molecule 21: Nuclear pore complex protein NUP54



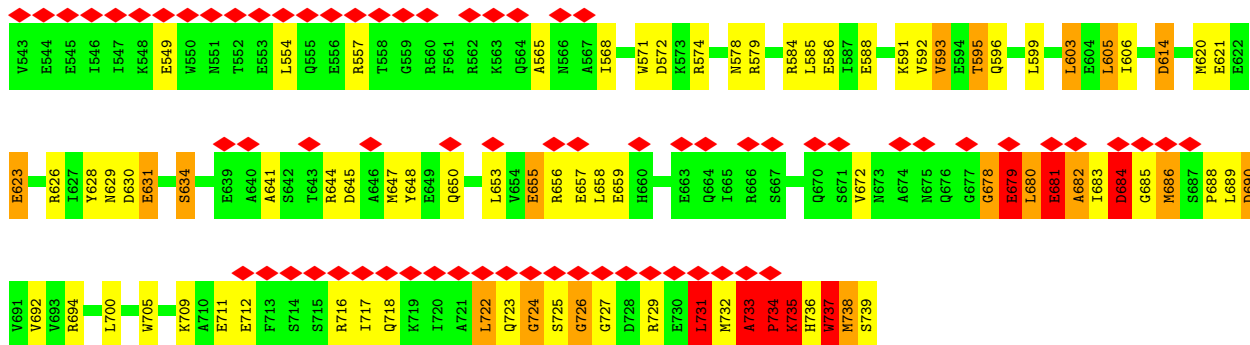
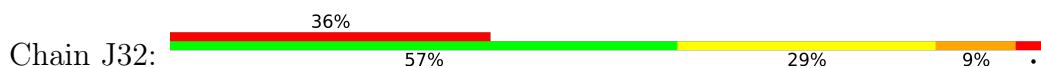
• Molecule 22: NUP58



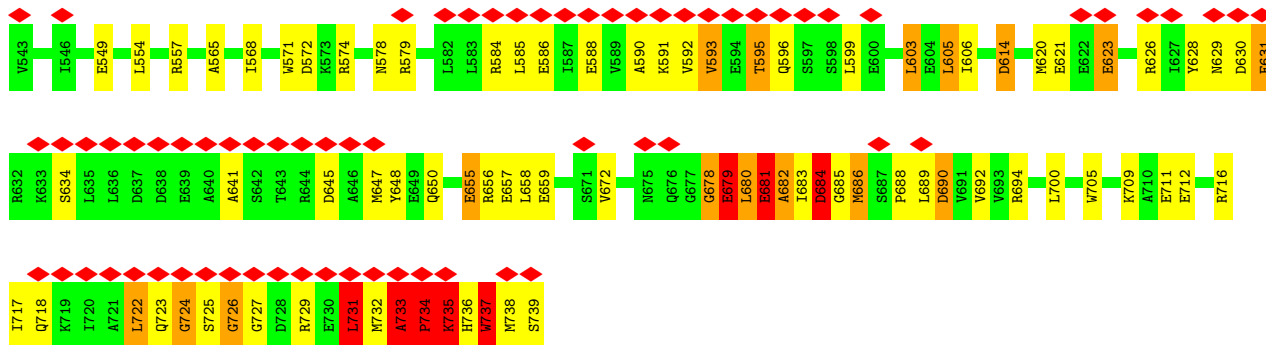




• Molecule 23: Nuclear pore complex protein NUP62

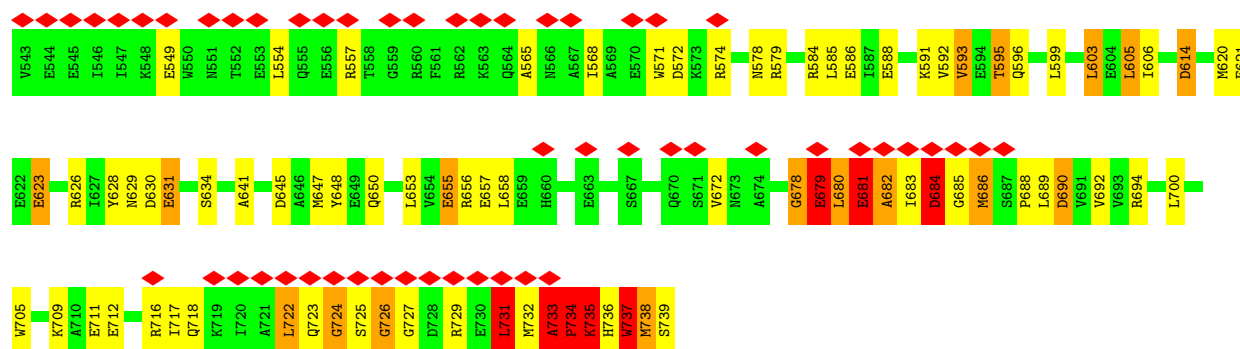


• Molecule 23: Nuclear pore complex protein NUP62

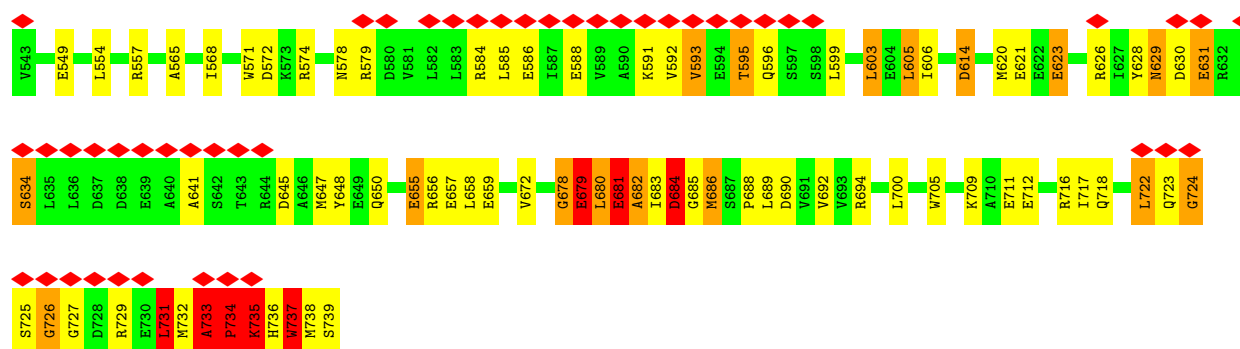


• Molecule 23: Nuclear pore complex protein NUP62

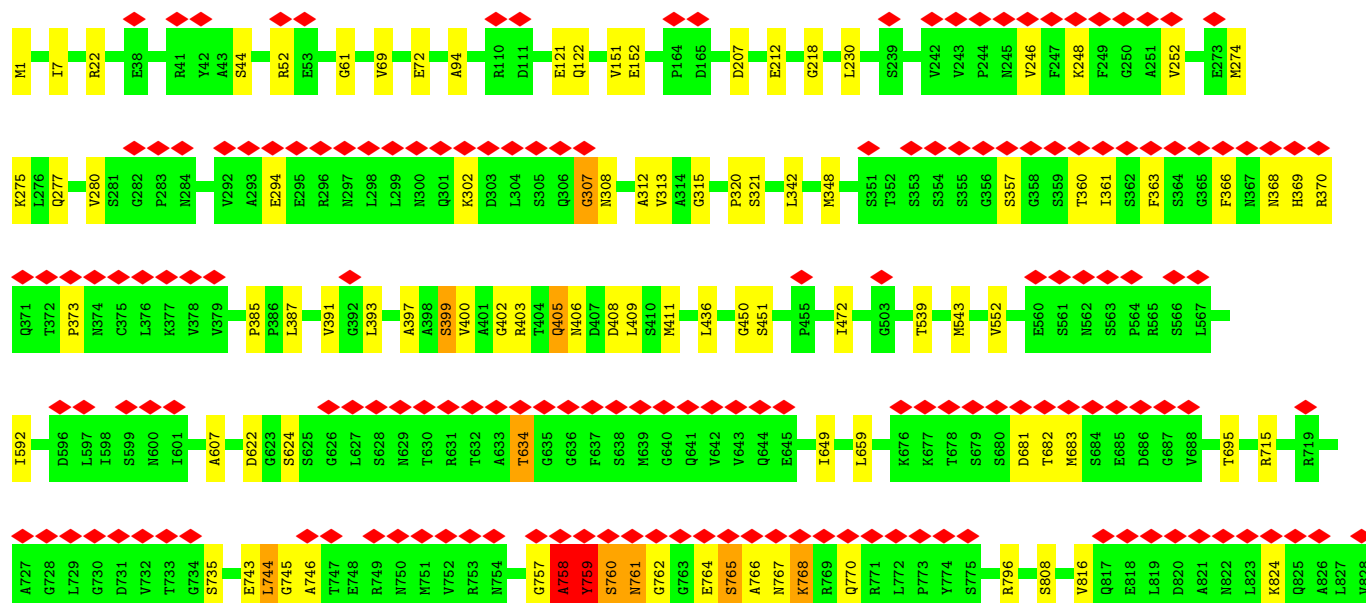
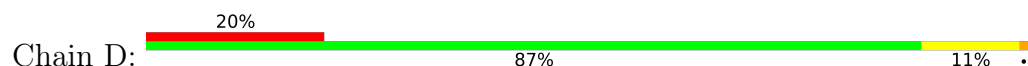


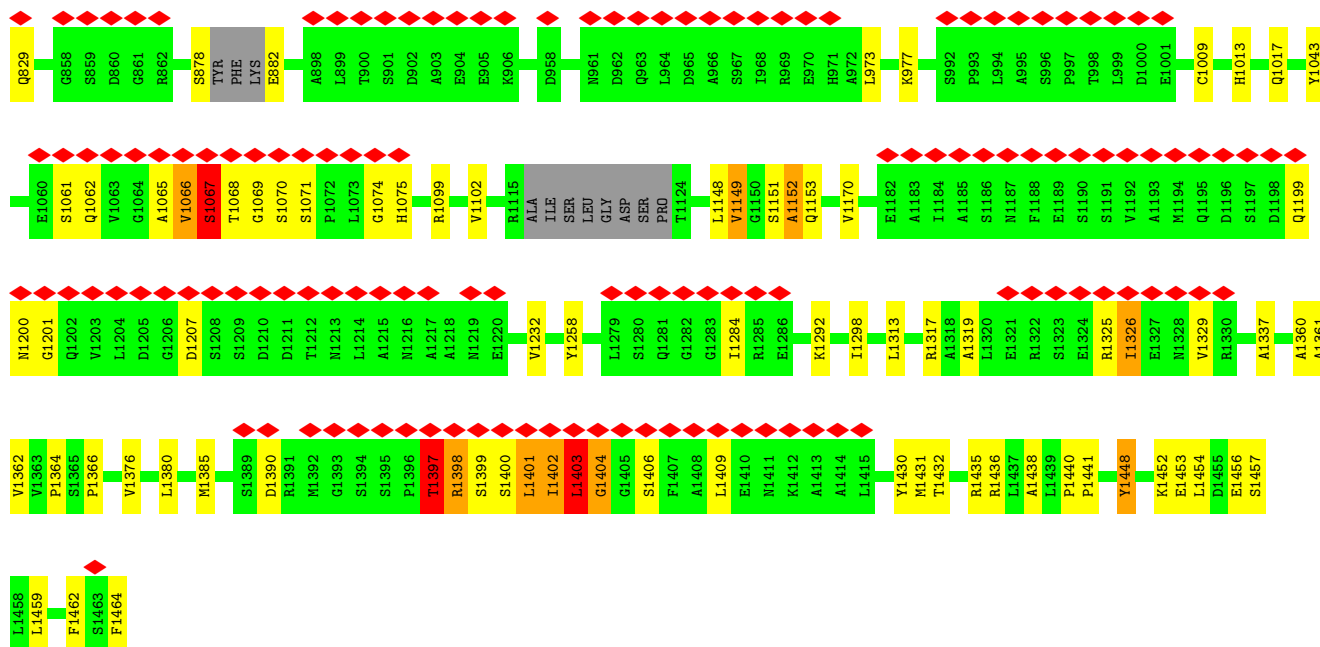


• Molecule 23: Nuclear pore complex protein NUP62

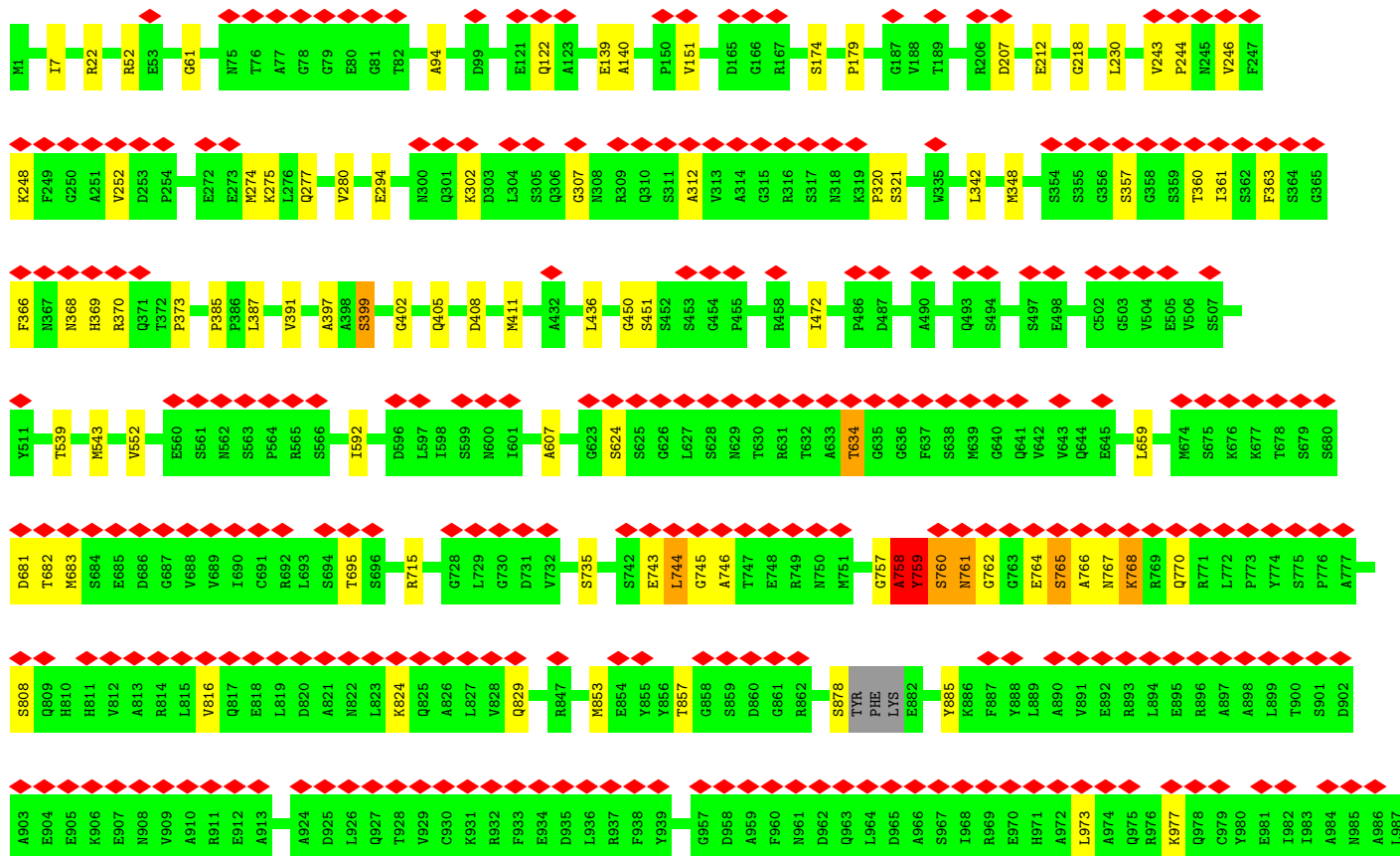
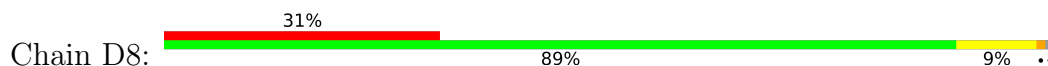


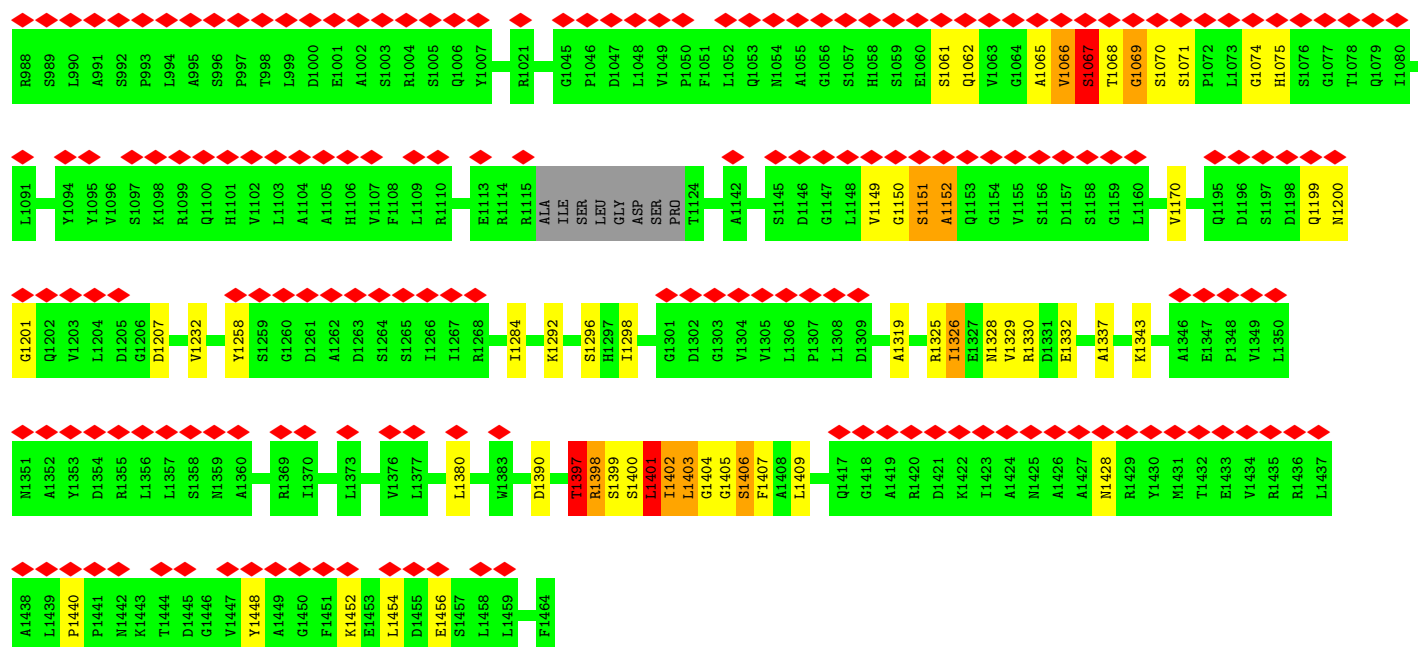
• Molecule 24: Nuclear pore complex protein NUP155



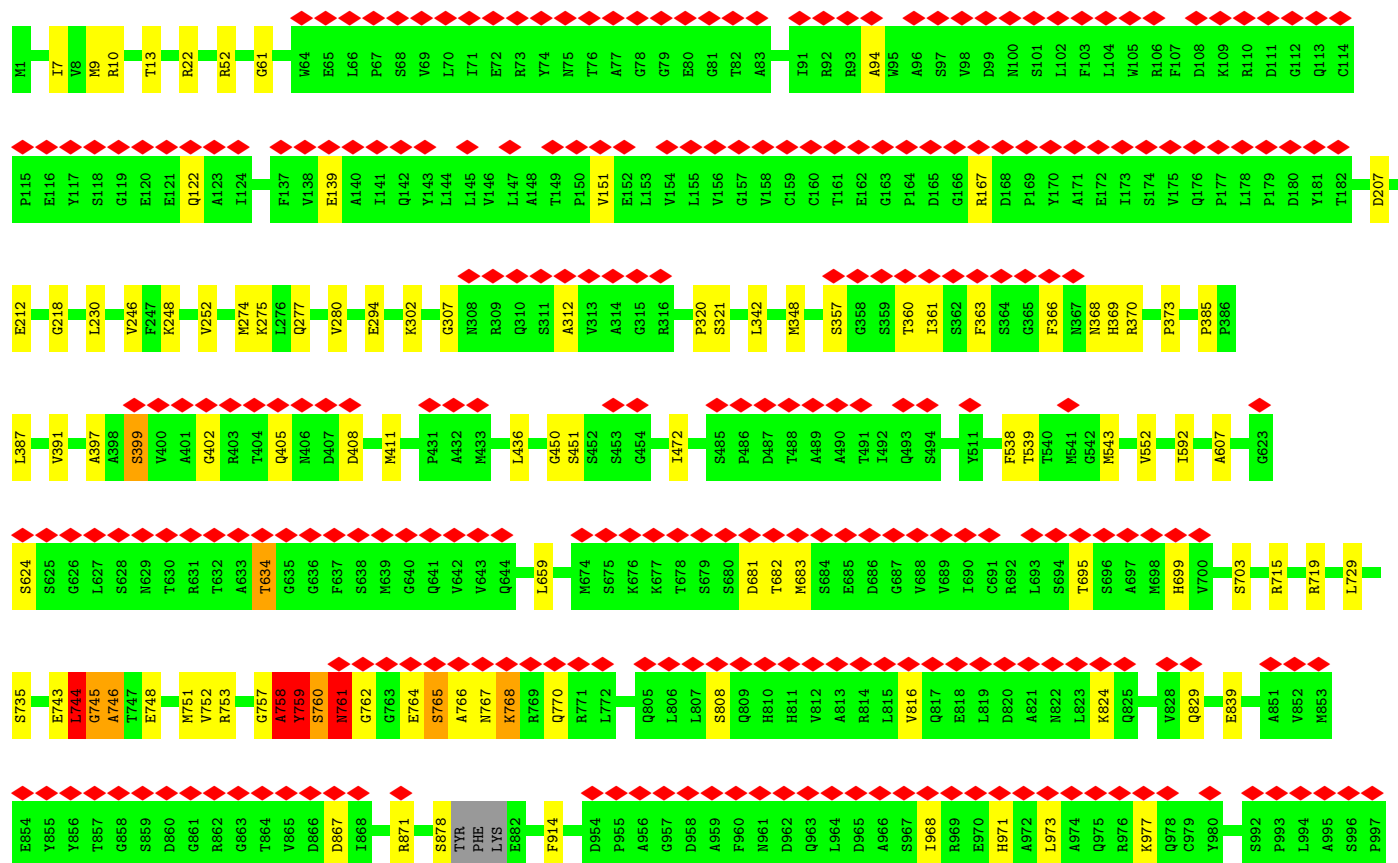
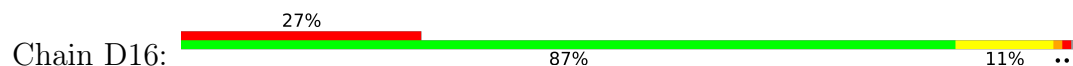


● Molecule 24: Nuclear pore complex protein NUP155

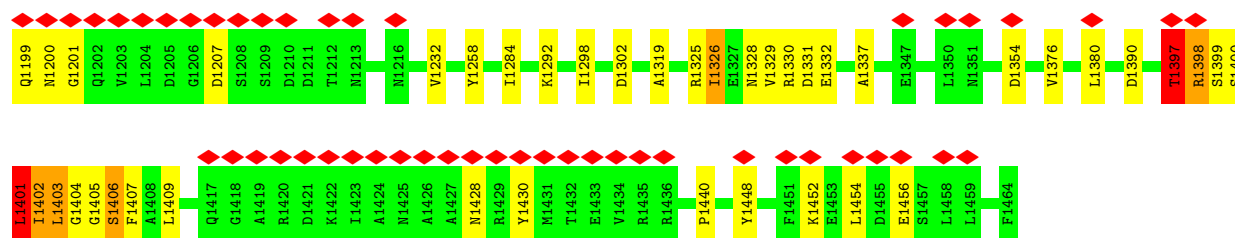




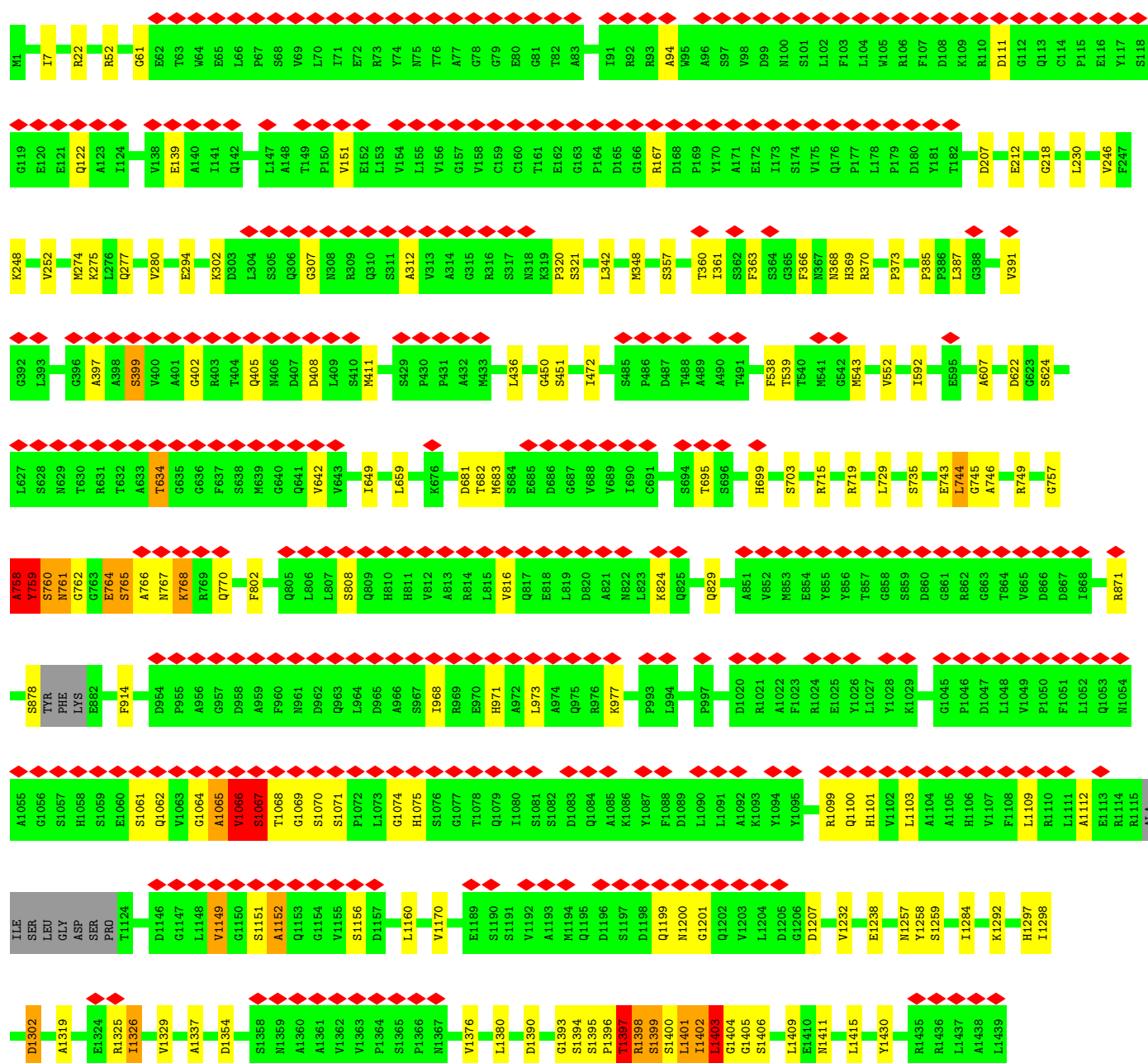
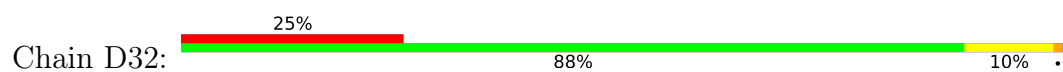
● Molecule 24: Nuclear pore complex protein NUP155

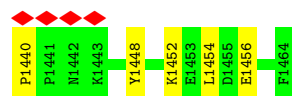






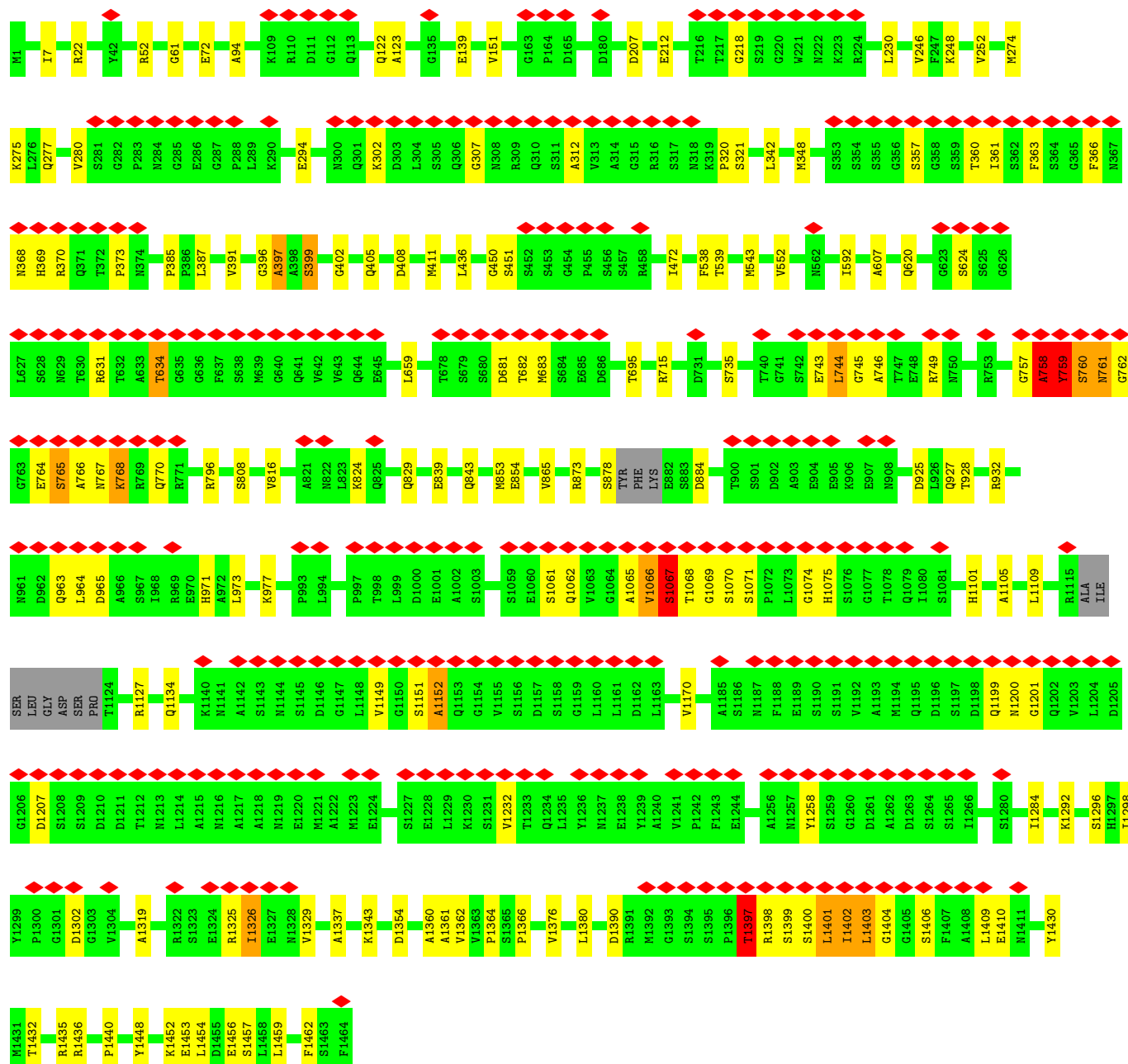
• Molecule 24: Nuclear pore complex protein NUP155





● Molecule 24: Nuclear pore complex protein NUP155

Chain D40: 21% 87% 11% ..



## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING         | Depositor |
| Imposed symmetry                     | POINT, C8                     | Depositor |
| Number of subtomograms used          | 75                            | Depositor |
| Resolution determination method      | OTHER                         | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY           | Depositor |
| Microscope                           | TFS KRIOS                     | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 130                           | Depositor |
| Minimum defocus (nm)                 | 2500                          | Depositor |
| Maximum defocus (nm)                 | 5000                          | Depositor |
| Magnification                        | Not provided                  |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 0.380                         | Depositor |
| Minimum map value                    | -0.333                        | Depositor |
| Average map value                    | 0.003                         | Depositor |
| Map value standard deviation         | 0.025                         | Depositor |
| Recommended contour level            | 0.07                          | Depositor |
| Map size ( $\text{\AA}$ )            | 1740.8, 1740.8, 1740.8        | wwPDB     |
| Map dimensions                       | 200, 200, 200                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 8.704, 8.704, 8.704           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 1   | R     | 2.22         | 73/11843 (0.6%)  | 1.56        | 85/16033 (0.5%)  |
| 1   | R16   | 2.21         | 73/11843 (0.6%)  | 1.56        | 84/16033 (0.5%)  |
| 1   | R8    | 2.22         | 73/11843 (0.6%)  | 1.56        | 81/16033 (0.5%)  |
| 2   | M     | 1.26         | 111/5730 (1.9%)  | 1.42        | 99/7766 (1.3%)   |
| 2   | M16   | 1.26         | 114/5730 (2.0%)  | 1.42        | 97/7766 (1.2%)   |
| 2   | M8    | 1.26         | 111/5730 (1.9%)  | 1.42        | 97/7766 (1.2%)   |
| 3   | N     | 1.24         | 41/2366 (1.7%)   | 1.32        | 25/3234 (0.8%)   |
| 3   | N16   | 1.24         | 39/2366 (1.6%)   | 1.32        | 25/3234 (0.8%)   |
| 3   | N8    | 1.24         | 40/2366 (1.7%)   | 1.32        | 25/3234 (0.8%)   |
| 4   | T     | 3.67         | 6/5605 (0.1%)    | 1.68        | 19/7591 (0.3%)   |
| 4   | T16   | 3.67         | 6/5605 (0.1%)    | 1.68        | 17/7591 (0.2%)   |
| 4   | T8    | 3.67         | 6/5605 (0.1%)    | 1.68        | 17/7591 (0.2%)   |
| 5   | P     | 1.26         | 106/5736 (1.8%)  | 1.29        | 85/7754 (1.1%)   |
| 5   | P16   | 1.26         | 105/5736 (1.8%)  | 1.29        | 85/7754 (1.1%)   |
| 5   | P8    | 1.26         | 107/5736 (1.9%)  | 1.29        | 85/7754 (1.1%)   |
| 6   | O     | 1.17         | 33/2391 (1.4%)   | 1.30        | 34/3246 (1.0%)   |
| 6   | O16   | 1.16         | 33/2391 (1.4%)   | 1.30        | 34/3246 (1.0%)   |
| 6   | O8    | 1.17         | 33/2391 (1.4%)   | 1.30        | 34/3246 (1.0%)   |
| 7   | Q     | 1.29         | 51/2834 (1.8%)   | 1.48        | 53/3849 (1.4%)   |
| 7   | Q16   | 1.29         | 51/2834 (1.8%)   | 1.48        | 53/3849 (1.4%)   |
| 7   | Q8    | 1.28         | 48/2834 (1.7%)   | 1.48        | 53/3849 (1.4%)   |
| 8   | L     | 2.52         | 4/7942 (0.1%)    | 1.52        | 13/10761 (0.1%)  |
| 8   | L16   | 2.52         | 3/7942 (0.0%)    | 1.52        | 13/10761 (0.1%)  |
| 8   | L8    | 2.52         | 3/7942 (0.0%)    | 1.52        | 13/10761 (0.1%)  |
| 9   | K     | 1.77         | 213/5800 (3.7%)  | 1.91        | 212/7828 (2.7%)  |
| 9   | K16   | 0.77         | 0/5801           | 1.25        | 6/7828 (0.1%)    |
| 9   | K8    | 1.77         | 215/5800 (3.7%)  | 1.91        | 211/7828 (2.7%)  |
| 10  | C     | 1.59         | 399/14649 (2.7%) | 1.80        | 503/19823 (2.5%) |
| 10  | C16   | 1.59         | 409/14783 (2.8%) | 1.82        | 520/20005 (2.6%) |
| 10  | C24   | 1.59         | 410/14783 (2.8%) | 1.82        | 526/20005 (2.6%) |
| 10  | C32   | 1.59         | 413/14783 (2.8%) | 1.82        | 525/20005 (2.6%) |
| 10  | C8    | 1.58         | 381/14420 (2.6%) | 1.73        | 454/19508 (2.3%) |
| 11  | A16   | 1.24         | 107/6584 (1.6%)  | 1.21        | 61/8878 (0.7%)   |
| 11  | A24   | 1.24         | 99/6584 (1.5%)   | 1.23        | 68/8878 (0.8%)   |

| Mol | Chain | Bond lengths |                    | Bond angles |                    |
|-----|-------|--------------|--------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5            | RMSZ        | # Z  >5            |
| 11  | A32   | 1.24         | 108/6584 (1.6%)    | 1.21        | 61/8878 (0.7%)     |
| 11  | A40   | 1.24         | 99/6584 (1.5%)     | 1.23        | 68/8878 (0.8%)     |
| 12  | A     | 1.23         | 84/5826 (1.4%)     | 1.21        | 58/7855 (0.7%)     |
| 12  | A48   | 1.23         | 86/5855 (1.5%)     | 1.21        | 58/7897 (0.7%)     |
| 13  | V     | 1.78         | 67/1617 (4.1%)     | 1.71        | 42/2175 (1.9%)     |
| 14  | W     | 1.13         | 65/6274 (1.0%)     | 1.36        | 70/8517 (0.8%)     |
| 15  | J     | 1.49         | 50/1516 (3.3%)     | 1.41        | 26/2038 (1.3%)     |
| 16  | A8    | 1.16         | 5/530 (0.9%)       | 1.38        | 10/709 (1.4%)      |
| 17  | F     | 1.44         | 6/220 (2.7%)       | 2.85        | 17/302 (5.6%)      |
| 17  | F16   | 1.45         | 6/220 (2.7%)       | 2.88        | 17/302 (5.6%)      |
| 17  | F24   | 1.45         | 6/220 (2.7%)       | 2.88        | 17/302 (5.6%)      |
| 17  | F8    | 1.44         | 6/220 (2.7%)       | 2.87        | 17/302 (5.6%)      |
| 18  | B     | 1.42         | 356/15710 (2.3%)   | 1.68        | 461/21300 (2.2%)   |
| 18  | B8    | 1.42         | 356/15710 (2.3%)   | 1.68        | 467/21300 (2.2%)   |
| 19  | 4     | 1.53         | 98/3497 (2.8%)     | 1.74        | 92/4746 (1.9%)     |
| 19  | 48    | 1.53         | 98/3497 (2.8%)     | 1.74        | 89/4746 (1.9%)     |
| 20  | E     | 1.51         | 95/4165 (2.3%)     | 1.56        | 92/5657 (1.6%)     |
| 20  | E8    | 1.51         | 95/4165 (2.3%)     | 1.56        | 91/5657 (1.6%)     |
| 21  | H     | 1.31         | 46/2046 (2.2%)     | 1.31        | 24/2749 (0.9%)     |
| 21  | H16   | 1.32         | 45/2046 (2.2%)     | 1.31        | 24/2749 (0.9%)     |
| 21  | H24   | 1.31         | 45/2046 (2.2%)     | 1.31        | 24/2749 (0.9%)     |
| 21  | H8    | 1.31         | 45/2046 (2.2%)     | 1.31        | 24/2749 (0.9%)     |
| 22  | I     | 1.45         | 50/1978 (2.5%)     | 1.35        | 33/2664 (1.2%)     |
| 22  | I16   | 1.45         | 50/1978 (2.5%)     | 1.34        | 32/2664 (1.2%)     |
| 22  | I24   | 1.45         | 48/1978 (2.4%)     | 1.34        | 33/2664 (1.2%)     |
| 22  | I8    | 1.45         | 51/1978 (2.6%)     | 1.34        | 31/2664 (1.2%)     |
| 23  | J16   | 1.30         | 30/1617 (1.9%)     | 1.42        | 39/2174 (1.8%)     |
| 23  | J24   | 1.30         | 29/1617 (1.8%)     | 1.42        | 39/2174 (1.8%)     |
| 23  | J32   | 1.30         | 31/1617 (1.9%)     | 1.41        | 39/2174 (1.8%)     |
| 23  | J8    | 1.30         | 31/1617 (1.9%)     | 1.42        | 39/2174 (1.8%)     |
| 24  | D     | 0.76         | 2/11328 (0.0%)     | 1.25        | 27/15333 (0.2%)    |
| 24  | D16   | 0.76         | 2/11328 (0.0%)     | 1.25        | 26/15333 (0.2%)    |
| 24  | D24   | 0.76         | 2/11328 (0.0%)     | 1.25        | 24/15333 (0.2%)    |
| 24  | D32   | 0.76         | 2/11328 (0.0%)     | 1.25        | 26/15333 (0.2%)    |
| 24  | D40   | 0.76         | 2/11328 (0.0%)     | 1.25        | 27/15333 (0.2%)    |
| 24  | D8    | 0.76         | 2/11328 (0.0%)     | 1.25        | 26/15333 (0.2%)    |
| All | All   | 1.65         | 6115/410270 (1.5%) | 1.52        | 6602/555195 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | R     | 0                   | 45                  |
| 1   | R16   | 0                   | 45                  |
| 1   | R8    | 0                   | 45                  |
| 2   | M     | 0                   | 33                  |
| 2   | M16   | 0                   | 34                  |
| 2   | M8    | 0                   | 33                  |
| 3   | N     | 0                   | 14                  |
| 3   | N16   | 0                   | 14                  |
| 3   | N8    | 0                   | 14                  |
| 4   | T     | 0                   | 7                   |
| 4   | T16   | 0                   | 7                   |
| 4   | T8    | 0                   | 7                   |
| 5   | P     | 0                   | 33                  |
| 5   | P16   | 0                   | 33                  |
| 5   | P8    | 0                   | 33                  |
| 6   | O     | 0                   | 9                   |
| 6   | O16   | 0                   | 9                   |
| 6   | O8    | 0                   | 9                   |
| 7   | Q     | 0                   | 17                  |
| 7   | Q16   | 0                   | 17                  |
| 7   | Q8    | 0                   | 17                  |
| 8   | L     | 0                   | 3                   |
| 8   | L16   | 0                   | 3                   |
| 8   | L8    | 0                   | 3                   |
| 9   | K     | 0                   | 84                  |
| 9   | K16   | 0                   | 6                   |
| 9   | K8    | 0                   | 84                  |
| 10  | C     | 0                   | 171                 |
| 10  | C16   | 0                   | 178                 |
| 10  | C24   | 0                   | 178                 |
| 10  | C32   | 0                   | 178                 |
| 10  | C8    | 0                   | 146                 |
| 11  | A16   | 0                   | 38                  |
| 11  | A24   | 0                   | 40                  |
| 11  | A32   | 0                   | 38                  |
| 11  | A40   | 0                   | 40                  |
| 12  | A     | 0                   | 36                  |
| 12  | A48   | 0                   | 36                  |
| 13  | V     | 0                   | 24                  |
| 14  | W     | 0                   | 22                  |
| 15  | J     | 0                   | 7                   |
| 16  | A8    | 0                   | 3                   |
| 17  | F     | 0                   | 10                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 17  | F16   | 0                   | 10                  |
| 17  | F24   | 0                   | 10                  |
| 17  | F8    | 0                   | 10                  |
| 18  | B     | 0                   | 196                 |
| 18  | B8    | 0                   | 198                 |
| 19  | 4     | 0                   | 43                  |
| 19  | 48    | 0                   | 43                  |
| 20  | E     | 0                   | 51                  |
| 20  | E8    | 0                   | 51                  |
| 21  | H     | 0                   | 8                   |
| 21  | H16   | 0                   | 8                   |
| 21  | H24   | 0                   | 8                   |
| 21  | H8    | 0                   | 8                   |
| 22  | I     | 0                   | 12                  |
| 22  | I16   | 0                   | 12                  |
| 22  | I24   | 0                   | 12                  |
| 22  | I8    | 0                   | 12                  |
| 23  | J16   | 0                   | 9                   |
| 23  | J24   | 0                   | 9                   |
| 23  | J32   | 0                   | 9                   |
| 23  | J8    | 0                   | 9                   |
| 24  | D     | 0                   | 29                  |
| 24  | D16   | 0                   | 29                  |
| 24  | D24   | 0                   | 29                  |
| 24  | D32   | 0                   | 29                  |
| 24  | D40   | 0                   | 29                  |
| 24  | D8    | 0                   | 29                  |
| All | All   | 0                   | 2705                |

All (6115) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | R     | 529  | HIS  | CD2-NE2 | 170.27 | 3.25        | 1.37     |
| 1   | R8    | 529  | HIS  | CD2-NE2 | 170.21 | 3.25        | 1.37     |
| 1   | R16   | 529  | HIS  | CD2-NE2 | 170.14 | 3.25        | 1.37     |
| 4   | T     | 160  | HIS  | CD2-NE2 | 169.95 | 3.24        | 1.37     |
| 4   | T8    | 160  | HIS  | CD2-NE2 | 169.94 | 3.24        | 1.37     |
| 4   | T16   | 160  | HIS  | CD2-NE2 | 169.85 | 3.24        | 1.37     |
| 8   | L16   | 1054 | HIS  | CD2-NE2 | 169.36 | 3.24        | 1.37     |
| 8   | L8    | 1054 | HIS  | CD2-NE2 | 169.32 | 3.24        | 1.37     |
| 8   | L     | 1054 | HIS  | CD2-NE2 | 169.25 | 3.24        | 1.37     |
| 8   | L8    | 1054 | HIS  | CE1-NE2 | 124.57 | 2.57        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 8   | L     | 1054 | HIS  | CE1-NE2 | 124.54 | 2.57        | 1.32     |
| 8   | L16   | 1054 | HIS  | CE1-NE2 | 124.51 | 2.57        | 1.32     |
| 4   | T16   | 386  | HIS  | CE1-NE2 | 123.52 | 2.56        | 1.32     |
| 4   | T     | 386  | HIS  | CE1-NE2 | 123.48 | 2.56        | 1.32     |
| 4   | T8    | 386  | HIS  | CE1-NE2 | 123.46 | 2.56        | 1.32     |
| 1   | R16   | 529  | HIS  | CE1-NE2 | 122.75 | 2.55        | 1.32     |
| 1   | R     | 529  | HIS  | CE1-NE2 | 122.70 | 2.55        | 1.32     |
| 1   | R8    | 529  | HIS  | CE1-NE2 | 122.68 | 2.55        | 1.32     |
| 4   | T     | 160  | HIS  | CE1-NE2 | 122.62 | 2.55        | 1.32     |
| 4   | T16   | 160  | HIS  | CE1-NE2 | 122.59 | 2.55        | 1.32     |
| 4   | T8    | 160  | HIS  | CE1-NE2 | 122.49 | 2.55        | 1.32     |
| 4   | T16   | 386  | HIS  | ND1-CE1 | 82.06  | 2.14        | 1.32     |
| 4   | T     | 386  | HIS  | ND1-CE1 | 82.05  | 2.14        | 1.32     |
| 4   | T8    | 386  | HIS  | ND1-CE1 | 81.96  | 2.14        | 1.32     |
| 4   | T     | 386  | HIS  | CD2-NE2 | 69.03  | 2.13        | 1.37     |
| 4   | T8    | 386  | HIS  | CD2-NE2 | 68.92  | 2.13        | 1.37     |
| 4   | T16   | 386  | HIS  | CD2-NE2 | 68.87  | 2.13        | 1.37     |
| 1   | R16   | 1121 | ARG  | C-N     | 38.47  | 1.87        | 1.33     |
| 1   | R     | 1121 | ARG  | C-N     | 38.45  | 1.87        | 1.33     |
| 1   | R8    | 1121 | ARG  | C-N     | 38.38  | 1.87        | 1.33     |
| 10  | C16   | 668  | ALA  | C-N     | 34.24  | 1.83        | 1.33     |
| 10  | C24   | 668  | ALA  | C-N     | 34.22  | 1.83        | 1.33     |
| 10  | C8    | 668  | ALA  | C-N     | 34.20  | 1.83        | 1.33     |
| 10  | C     | 668  | ALA  | C-N     | 34.15  | 1.83        | 1.33     |
| 10  | C32   | 668  | ALA  | C-N     | 34.15  | 1.83        | 1.33     |
| 1   | R     | 529  | HIS  | ND1-CE1 | -31.16 | 1.01        | 1.32     |
| 4   | T8    | 160  | HIS  | ND1-CE1 | -31.16 | 1.01        | 1.32     |
| 4   | T     | 160  | HIS  | ND1-CE1 | -31.12 | 1.01        | 1.32     |
| 1   | R8    | 529  | HIS  | ND1-CE1 | -31.09 | 1.01        | 1.32     |
| 8   | L16   | 1054 | HIS  | ND1-CE1 | -31.09 | 1.01        | 1.32     |
| 1   | R16   | 529  | HIS  | ND1-CE1 | -31.08 | 1.01        | 1.32     |
| 8   | L8    | 1054 | HIS  | ND1-CE1 | -31.08 | 1.01        | 1.32     |
| 4   | T16   | 160  | HIS  | ND1-CE1 | -31.04 | 1.01        | 1.32     |
| 8   | L     | 1054 | HIS  | ND1-CE1 | -30.88 | 1.01        | 1.32     |
| 20  | E8    | 340  | GLY  | C-N     | 25.05  | 1.67        | 1.33     |
| 20  | E     | 340  | GLY  | C-N     | 25.04  | 1.67        | 1.33     |
| 9   | K8    | 719  | GLY  | C-N     | 24.76  | 1.74        | 1.33     |
| 9   | K     | 719  | GLY  | C-N     | 24.73  | 1.74        | 1.33     |
| 14  | W     | 584  | CYS  | C-N     | 24.32  | 1.66        | 1.33     |
| 10  | C     | 670  | GLU  | C-N     | 21.34  | 1.67        | 1.33     |
| 10  | C8    | 670  | GLU  | C-N     | 21.31  | 1.67        | 1.33     |
| 10  | C16   | 670  | GLU  | C-N     | 21.31  | 1.67        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C32   | 670  | GLU  | C-N   | 21.30  | 1.67        | 1.33     |
| 10  | C24   | 670  | GLU  | C-N   | 21.27  | 1.67        | 1.33     |
| 10  | C24   | 666  | LEU  | C-N   | 19.82  | 1.57        | 1.33     |
| 10  | C16   | 666  | LEU  | C-N   | 19.76  | 1.57        | 1.33     |
| 10  | C32   | 666  | LEU  | C-N   | 19.72  | 1.57        | 1.33     |
| 10  | C8    | 666  | LEU  | C-N   | 19.68  | 1.57        | 1.33     |
| 10  | C     | 666  | LEU  | C-N   | 19.66  | 1.57        | 1.33     |
| 9   | K     | 1048 | GLN  | C-N   | 19.08  | 1.59        | 1.34     |
| 9   | K8    | 1048 | GLN  | C-N   | 19.07  | 1.59        | 1.34     |
| 20  | E     | 429  | PRO  | C-N   | 18.92  | 1.63        | 1.33     |
| 20  | E8    | 429  | PRO  | C-N   | 18.86  | 1.63        | 1.33     |
| 9   | K     | 1273 | GLU  | C-N   | 18.83  | 1.60        | 1.33     |
| 9   | K8    | 1273 | GLU  | C-N   | 18.81  | 1.60        | 1.33     |
| 18  | B8    | 540  | ILE  | C-N   | 18.68  | 1.58        | 1.33     |
| 18  | B     | 540  | ILE  | C-N   | 18.62  | 1.58        | 1.33     |
| 10  | C24   | 1837 | CYS  | C-N   | 18.59  | 1.59        | 1.33     |
| 10  | C32   | 1837 | CYS  | C-N   | 18.59  | 1.59        | 1.33     |
| 10  | C8    | 1837 | CYS  | C-N   | 18.57  | 1.59        | 1.33     |
| 10  | C     | 1837 | CYS  | C-N   | 18.55  | 1.59        | 1.33     |
| 10  | C16   | 1837 | CYS  | C-N   | 18.51  | 1.59        | 1.33     |
| 9   | K8    | 1271 | GLU  | C-N   | 17.72  | 1.56        | 1.33     |
| 9   | K     | 1271 | GLU  | C-N   | 17.65  | 1.56        | 1.33     |
| 9   | K     | 1269 | CYS  | C-N   | 16.64  | 1.54        | 1.33     |
| 9   | K8    | 1269 | CYS  | C-N   | 16.58  | 1.54        | 1.33     |
| 10  | C24   | 1130 | SER  | C-N   | 16.47  | 1.57        | 1.33     |
| 10  | C16   | 1130 | SER  | C-N   | 16.45  | 1.57        | 1.33     |
| 10  | C     | 1130 | SER  | C-N   | 16.43  | 1.57        | 1.33     |
| 10  | C32   | 1130 | SER  | C-N   | 16.30  | 1.57        | 1.33     |
| 9   | K8    | 1275 | ILE  | C-N   | 16.27  | 1.55        | 1.33     |
| 9   | K     | 1275 | ILE  | C-N   | 16.26  | 1.55        | 1.33     |
| 10  | C8    | 1130 | SER  | C-N   | 16.25  | 1.57        | 1.33     |
| 10  | C32   | 1358 | ASP  | C-N   | 16.16  | 1.55        | 1.33     |
| 10  | C8    | 1358 | ASP  | C-N   | 16.15  | 1.55        | 1.33     |
| 10  | C16   | 1358 | ASP  | C-N   | 16.12  | 1.55        | 1.33     |
| 10  | C24   | 1358 | ASP  | C-N   | 16.11  | 1.55        | 1.33     |
| 10  | C     | 1358 | ASP  | C-N   | 16.06  | 1.55        | 1.33     |
| 9   | K8    | 927  | ARG  | C-N   | 16.01  | 1.54        | 1.33     |
| 9   | K     | 927  | ARG  | C-N   | 15.99  | 1.54        | 1.33     |
| 9   | K     | 721  | PRO  | C-N   | 15.58  | 1.52        | 1.33     |
| 9   | K8    | 721  | PRO  | C-N   | 15.52  | 1.52        | 1.33     |
| 9   | K8    | 1051 | GLU  | C-N   | -15.37 | 1.12        | 1.33     |
| 9   | K     | 1051 | GLU  | C-N   | -15.27 | 1.12        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C8    | 250  | GLU  | C-N   | 15.05  | 1.41        | 1.33     |
| 10  | C8    | 1656 | VAL  | C-N   | 15.03  | 1.54        | 1.33     |
| 10  | C32   | 1656 | VAL  | C-N   | 14.91  | 1.54        | 1.33     |
| 10  | C32   | 250  | GLU  | C-N   | 14.91  | 1.41        | 1.33     |
| 20  | E     | 342  | GLN  | C-N   | 14.90  | 1.57        | 1.33     |
| 10  | C     | 1656 | VAL  | C-N   | 14.90  | 1.54        | 1.33     |
| 10  | C24   | 1656 | VAL  | C-N   | 14.89  | 1.54        | 1.33     |
| 20  | E8    | 342  | GLN  | C-N   | 14.89  | 1.57        | 1.33     |
| 10  | C16   | 1656 | VAL  | C-N   | 14.85  | 1.54        | 1.33     |
| 10  | C16   | 250  | GLU  | C-N   | 14.80  | 1.41        | 1.33     |
| 10  | C     | 250  | GLU  | C-N   | 14.75  | 1.41        | 1.33     |
| 14  | W     | 610  | PRO  | C-N   | -14.62 | 1.14        | 1.34     |
| 10  | C24   | 250  | GLU  | C-N   | 14.56  | 1.41        | 1.33     |
| 10  | C32   | 882  | GLY  | C-N   | 14.23  | 1.52        | 1.33     |
| 10  | C16   | 882  | GLY  | C-N   | 14.22  | 1.52        | 1.33     |
| 10  | C24   | 882  | GLY  | C-N   | 14.19  | 1.52        | 1.33     |
| 10  | C8    | 882  | GLY  | C-N   | 14.19  | 1.52        | 1.33     |
| 18  | B     | 1961 | TYR  | C-N   | 14.15  | 1.50        | 1.33     |
| 10  | C     | 450  | PRO  | C-N   | 14.12  | 1.53        | 1.33     |
| 10  | C     | 882  | GLY  | C-N   | 14.09  | 1.52        | 1.33     |
| 18  | B8    | 1961 | TYR  | C-N   | 14.08  | 1.50        | 1.33     |
| 10  | C24   | 450  | PRO  | C-N   | 14.07  | 1.53        | 1.33     |
| 10  | C16   | 450  | PRO  | C-N   | 14.02  | 1.53        | 1.33     |
| 10  | C32   | 450  | PRO  | C-N   | 14.02  | 1.53        | 1.33     |
| 10  | C8    | 450  | PRO  | C-N   | 14.02  | 1.53        | 1.33     |
| 10  | C8    | 1624 | LEU  | C-N   | -13.87 | 1.14        | 1.33     |
| 10  | C32   | 1624 | LEU  | C-N   | -13.87 | 1.14        | 1.33     |
| 10  | C     | 1624 | LEU  | C-N   | -13.81 | 1.14        | 1.33     |
| 10  | C16   | 1624 | LEU  | C-N   | -13.78 | 1.14        | 1.33     |
| 10  | C24   | 1624 | LEU  | C-N   | -13.75 | 1.14        | 1.33     |
| 18  | B8    | 853  | HIS  | C-N   | 13.70  | 1.49        | 1.33     |
| 18  | B     | 853  | HIS  | C-N   | 13.68  | 1.49        | 1.33     |
| 10  | C32   | 1332 | GLN  | C-N   | -13.64 | 1.18        | 1.33     |
| 10  | C32   | 18   | THR  | C-N   | 13.63  | 1.52        | 1.33     |
| 10  | C16   | 1332 | GLN  | C-N   | -13.62 | 1.18        | 1.33     |
| 10  | C24   | 18   | THR  | C-N   | 13.61  | 1.52        | 1.33     |
| 10  | C     | 1332 | GLN  | C-N   | -13.59 | 1.18        | 1.33     |
| 10  | C8    | 18   | THR  | C-N   | 13.57  | 1.52        | 1.33     |
| 10  | C16   | 18   | THR  | C-N   | 13.57  | 1.52        | 1.33     |
| 10  | C     | 18   | THR  | C-N   | 13.55  | 1.52        | 1.33     |
| 10  | C24   | 1332 | GLN  | C-N   | -13.54 | 1.18        | 1.33     |
| 10  | C8    | 1332 | GLN  | C-N   | -13.53 | 1.18        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C8    | 1366 | GLN  | C-N   | -13.40 | 1.16        | 1.33     |
| 10  | C24   | 1366 | GLN  | C-N   | -13.35 | 1.16        | 1.33     |
| 10  | C24   | 1615 | PHE  | C-N   | 13.34  | 1.48        | 1.33     |
| 10  | C32   | 1366 | GLN  | C-N   | -13.34 | 1.16        | 1.33     |
| 10  | C     | 1366 | GLN  | C-N   | -13.32 | 1.16        | 1.33     |
| 10  | C16   | 1366 | GLN  | C-N   | -13.31 | 1.16        | 1.33     |
| 10  | C     | 1615 | PHE  | C-N   | 13.27  | 1.48        | 1.33     |
| 18  | B8    | 1782 | CYS  | C-N   | 13.27  | 1.51        | 1.33     |
| 18  | B     | 1782 | CYS  | C-N   | 13.20  | 1.51        | 1.33     |
| 10  | C8    | 1615 | PHE  | C-N   | 13.19  | 1.48        | 1.33     |
| 10  | C32   | 1615 | PHE  | C-N   | 13.19  | 1.48        | 1.33     |
| 10  | C16   | 1615 | PHE  | C-N   | 13.16  | 1.48        | 1.33     |
| 13  | V     | 807  | LYS  | C-N   | -13.10 | 1.17        | 1.33     |
| 1   | R16   | 1388 | GLY  | C-N   | -13.00 | 1.15        | 1.33     |
| 10  | C24   | 1287 | MET  | C-N   | -12.96 | 1.18        | 1.33     |
| 10  | C16   | 1544 | GLY  | C-N   | 12.95  | 1.53        | 1.33     |
| 1   | R     | 1388 | GLY  | C-N   | -12.94 | 1.15        | 1.33     |
| 10  | C32   | 1544 | GLY  | C-N   | 12.92  | 1.53        | 1.33     |
| 1   | R8    | 1388 | GLY  | C-N   | -12.92 | 1.15        | 1.33     |
| 10  | C16   | 712  | LEU  | C-N   | 12.92  | 1.51        | 1.34     |
| 10  | C24   | 1544 | GLY  | C-N   | 12.92  | 1.53        | 1.33     |
| 10  | C16   | 1287 | MET  | C-N   | -12.91 | 1.18        | 1.33     |
| 10  | C32   | 712  | LEU  | C-N   | 12.90  | 1.51        | 1.34     |
| 10  | C8    | 1544 | GLY  | C-N   | 12.88  | 1.53        | 1.33     |
| 10  | C24   | 1073 | GLY  | C-N   | 12.88  | 1.50        | 1.33     |
| 10  | C32   | 1287 | MET  | C-N   | -12.88 | 1.18        | 1.33     |
| 10  | C16   | 1063 | PRO  | C-N   | -12.86 | 1.15        | 1.33     |
| 10  | C24   | 1063 | PRO  | C-N   | -12.86 | 1.15        | 1.33     |
| 10  | C8    | 1287 | MET  | C-N   | -12.86 | 1.18        | 1.33     |
| 10  | C     | 1287 | MET  | C-N   | -12.85 | 1.18        | 1.33     |
| 10  | C     | 712  | LEU  | C-N   | 12.84  | 1.51        | 1.34     |
| 10  | C24   | 712  | LEU  | C-N   | 12.84  | 1.51        | 1.34     |
| 10  | C     | 1063 | PRO  | C-N   | -12.83 | 1.15        | 1.33     |
| 10  | C     | 1536 | VAL  | C-N   | 12.78  | 1.51        | 1.33     |
| 10  | C     | 285  | MET  | C-N   | 12.78  | 1.49        | 1.33     |
| 10  | C32   | 1063 | PRO  | C-N   | -12.78 | 1.15        | 1.33     |
| 10  | C16   | 1073 | GLY  | C-N   | 12.77  | 1.50        | 1.33     |
| 10  | C8    | 1063 | PRO  | C-N   | -12.73 | 1.15        | 1.33     |
| 10  | C8    | 712  | LEU  | C-N   | 12.73  | 1.51        | 1.34     |
| 10  | C32   | 285  | MET  | C-N   | 12.72  | 1.49        | 1.33     |
| 10  | C24   | 285  | MET  | C-N   | 12.68  | 1.49        | 1.33     |
| 9   | K     | 1270 | VAL  | C-N   | -12.67 | 1.16        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C16   | 285  | MET  | C-N   | 12.67  | 1.49        | 1.33     |
| 10  | C32   | 1073 | GLY  | C-N   | 12.66  | 1.50        | 1.33     |
| 10  | C     | 1073 | GLY  | C-N   | 12.66  | 1.50        | 1.33     |
| 19  | 48    | 191  | GLY  | C-N   | 12.65  | 1.51        | 1.33     |
| 9   | K8    | 1270 | VAL  | C-N   | -12.64 | 1.16        | 1.33     |
| 19  | 4     | 191  | GLY  | C-N   | 12.63  | 1.51        | 1.33     |
| 10  | C8    | 1073 | GLY  | C-N   | 12.63  | 1.50        | 1.33     |
| 10  | C8    | 285  | MET  | C-N   | 12.60  | 1.49        | 1.33     |
| 10  | C24   | 1536 | VAL  | C-N   | 12.59  | 1.51        | 1.33     |
| 10  | C32   | 602  | VAL  | C-N   | 12.58  | 1.51        | 1.34     |
| 10  | C16   | 602  | VAL  | C-N   | 12.54  | 1.51        | 1.34     |
| 10  | C     | 602  | VAL  | C-N   | 12.53  | 1.51        | 1.34     |
| 19  | 48    | 198  | GLY  | C-N   | -12.53 | 1.15        | 1.33     |
| 10  | C24   | 1494 | ILE  | C-N   | 12.51  | 1.49        | 1.33     |
| 10  | C8    | 602  | VAL  | C-N   | 12.51  | 1.51        | 1.34     |
| 10  | C32   | 1536 | VAL  | C-N   | 12.51  | 1.51        | 1.33     |
| 19  | 4     | 198  | GLY  | C-N   | -12.50 | 1.15        | 1.33     |
| 10  | C16   | 1536 | VAL  | C-N   | 12.48  | 1.51        | 1.33     |
| 10  | C32   | 1494 | ILE  | C-N   | 12.47  | 1.49        | 1.33     |
| 18  | B     | 1251 | GLY  | C-N   | 12.46  | 1.51        | 1.33     |
| 10  | C8    | 1536 | VAL  | C-N   | 12.45  | 1.51        | 1.33     |
| 18  | B8    | 1251 | GLY  | C-N   | 12.45  | 1.51        | 1.33     |
| 10  | C16   | 1494 | ILE  | C-N   | 12.45  | 1.49        | 1.33     |
| 10  | C24   | 602  | VAL  | C-N   | 12.44  | 1.51        | 1.34     |
| 9   | K8    | 1218 | ARG  | C-N   | -12.39 | 1.18        | 1.34     |
| 10  | C     | 1494 | ILE  | C-N   | 12.36  | 1.49        | 1.33     |
| 9   | K     | 1218 | ARG  | C-N   | -12.36 | 1.18        | 1.34     |
| 9   | K8    | 1052 | SER  | C-N   | 12.36  | 1.50        | 1.33     |
| 9   | K     | 1052 | SER  | C-N   | 12.35  | 1.50        | 1.33     |
| 10  | C8    | 1494 | ILE  | C-N   | 12.34  | 1.49        | 1.33     |
| 9   | K8    | 1222 | PHE  | C-N   | 12.28  | 1.51        | 1.33     |
| 18  | B     | 852  | THR  | C-N   | 12.27  | 1.50        | 1.34     |
| 9   | K     | 1222 | PHE  | C-N   | 12.24  | 1.51        | 1.33     |
| 14  | W     | 588  | LYS  | C-N   | -12.21 | 1.16        | 1.33     |
| 18  | B8    | 852  | THR  | C-N   | 12.20  | 1.50        | 1.34     |
| 10  | C32   | 1538 | THR  | C-N   | 12.16  | 1.52        | 1.33     |
| 10  | C24   | 1538 | THR  | C-N   | 12.14  | 1.52        | 1.33     |
| 1   | R16   | 1494 | THR  | C-N   | 12.12  | 1.50        | 1.33     |
| 10  | C24   | 1333 | HIS  | C-N   | 12.12  | 1.50        | 1.34     |
| 18  | B8    | 1809 | SER  | C-N   | 12.12  | 1.47        | 1.33     |
| 18  | B     | 299  | CYS  | C-N   | -12.10 | 1.20        | 1.34     |
| 1   | R     | 1494 | THR  | C-N   | 12.10  | 1.50        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C     | 1333 | HIS  | C-N   | 12.10  | 1.50        | 1.34     |
| 10  | C16   | 1538 | THR  | C-N   | 12.09  | 1.52        | 1.33     |
| 1   | R8    | 1494 | THR  | C-N   | 12.08  | 1.50        | 1.33     |
| 18  | B8    | 299  | CYS  | C-N   | -12.08 | 1.20        | 1.34     |
| 10  | C16   | 1333 | HIS  | C-N   | 12.07  | 1.50        | 1.34     |
| 10  | C8    | 1777 | SER  | C-N   | -12.06 | 1.19        | 1.33     |
| 10  | C8    | 1333 | HIS  | C-N   | 12.05  | 1.50        | 1.34     |
| 10  | C8    | 1538 | THR  | C-N   | 12.04  | 1.52        | 1.33     |
| 10  | C32   | 1333 | HIS  | C-N   | 12.03  | 1.50        | 1.34     |
| 18  | B     | 1809 | SER  | C-N   | 12.02  | 1.47        | 1.33     |
| 10  | C32   | 69   | PRO  | N-CD  | -12.00 | 1.30        | 1.47     |
| 14  | W     | 647  | PRO  | N-CD  | -11.97 | 1.30        | 1.47     |
| 10  | C16   | 69   | PRO  | N-CD  | -11.96 | 1.30        | 1.47     |
| 10  | C     | 1777 | SER  | C-N   | -11.93 | 1.19        | 1.33     |
| 10  | C8    | 149  | PRO  | N-CD  | -11.92 | 1.31        | 1.47     |
| 10  | C24   | 65   | PRO  | N-CD  | -11.92 | 1.31        | 1.47     |
| 10  | C24   | 200  | GLY  | C-N   | 11.90  | 1.50        | 1.33     |
| 13  | V     | 731  | PRO  | N-CD  | -11.90 | 1.31        | 1.47     |
| 10  | C     | 69   | PRO  | N-CD  | -11.90 | 1.31        | 1.47     |
| 10  | C     | 149  | PRO  | N-CD  | -11.90 | 1.31        | 1.47     |
| 18  | B     | 1962 | PRO  | N-CD  | -11.89 | 1.31        | 1.47     |
| 10  | C16   | 149  | PRO  | N-CD  | -11.88 | 1.31        | 1.47     |
| 10  | C24   | 149  | PRO  | N-CD  | -11.87 | 1.31        | 1.47     |
| 10  | C16   | 1777 | SER  | C-N   | -11.86 | 1.19        | 1.33     |
| 10  | C8    | 200  | GLY  | C-N   | 11.86  | 1.50        | 1.33     |
| 10  | C32   | 149  | PRO  | N-CD  | -11.86 | 1.31        | 1.47     |
| 10  | C8    | 69   | PRO  | N-CD  | -11.86 | 1.31        | 1.47     |
| 10  | C32   | 47   | PRO  | N-CD  | -11.86 | 1.31        | 1.47     |
| 10  | C32   | 200  | GLY  | C-N   | 11.86  | 1.50        | 1.33     |
| 10  | C     | 200  | GLY  | C-N   | 11.84  | 1.50        | 1.33     |
| 10  | C24   | 69   | PRO  | N-CD  | -11.84 | 1.31        | 1.47     |
| 18  | B8    | 81   | PRO  | N-CD  | -11.84 | 1.31        | 1.47     |
| 10  | C8    | 923  | PRO  | N-CD  | -11.83 | 1.31        | 1.47     |
| 18  | B8    | 348  | PRO  | N-CD  | -11.83 | 1.31        | 1.47     |
| 10  | C32   | 1777 | SER  | C-N   | -11.83 | 1.19        | 1.33     |
| 10  | C32   | 65   | PRO  | N-CD  | -11.82 | 1.31        | 1.47     |
| 10  | C8    | 450  | PRO  | N-CD  | -11.82 | 1.31        | 1.47     |
| 10  | C16   | 65   | PRO  | N-CD  | -11.81 | 1.31        | 1.47     |
| 18  | B     | 348  | PRO  | N-CD  | -11.81 | 1.31        | 1.47     |
| 10  | C24   | 1777 | SER  | C-N   | -11.81 | 1.19        | 1.33     |
| 18  | B     | 81   | PRO  | N-CD  | -11.81 | 1.31        | 1.47     |
| 18  | B8    | 524  | GLU  | C-N   | -11.81 | 1.18        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 11  | A16   | 158  | PRO  | N-CD  | -11.81 | 1.31        | 1.47     |
| 14  | W     | 610  | PRO  | N-CD  | -11.80 | 1.31        | 1.47     |
| 14  | W     | 604  | PRO  | N-CD  | -11.80 | 1.31        | 1.47     |
| 5   | P     | 148  | PRO  | N-CD  | -11.79 | 1.31        | 1.47     |
| 10  | C16   | 200  | GLY  | C-N   | 11.79  | 1.50        | 1.33     |
| 1   | R     | 1182 | PRO  | N-CD  | -11.79 | 1.31        | 1.47     |
| 10  | C16   | 47   | PRO  | N-CD  | -11.79 | 1.31        | 1.47     |
| 12  | A48   | 158  | PRO  | N-CD  | -11.79 | 1.31        | 1.47     |
| 13  | V     | 751  | PRO  | N-CD  | -11.78 | 1.31        | 1.47     |
| 18  | B8    | 1962 | PRO  | N-CD  | -11.78 | 1.31        | 1.47     |
| 5   | P16   | 685  | PRO  | N-CD  | -11.78 | 1.31        | 1.47     |
| 10  | C8    | 65   | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 11  | A24   | 158  | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 11  | A40   | 158  | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 10  | C24   | 450  | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 10  | C     | 47   | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 10  | C     | 65   | PRO  | N-CD  | -11.77 | 1.31        | 1.47     |
| 10  | C24   | 47   | PRO  | N-CD  | -11.76 | 1.31        | 1.47     |
| 10  | C     | 450  | PRO  | N-CD  | -11.76 | 1.31        | 1.47     |
| 1   | R8    | 1182 | PRO  | N-CD  | -11.75 | 1.31        | 1.47     |
| 5   | P8    | 685  | PRO  | N-CD  | -11.74 | 1.31        | 1.47     |
| 10  | C8    | 47   | PRO  | N-CD  | -11.74 | 1.31        | 1.47     |
| 5   | P16   | 155  | PRO  | N-CD  | -11.73 | 1.31        | 1.47     |
| 1   | R16   | 1182 | PRO  | N-CD  | -11.73 | 1.31        | 1.47     |
| 5   | P8    | 155  | PRO  | N-CD  | -11.73 | 1.31        | 1.47     |
| 12  | A     | 158  | PRO  | N-CD  | -11.73 | 1.31        | 1.47     |
| 5   | P8    | 292  | GLU  | C-N   | -11.72 | 1.17        | 1.33     |
| 10  | C8    | 1726 | PRO  | N-CD  | -11.71 | 1.31        | 1.47     |
| 16  | A8    | 158  | PRO  | N-CD  | -11.71 | 1.31        | 1.47     |
| 10  | C16   | 450  | PRO  | N-CD  | -11.70 | 1.31        | 1.47     |
| 10  | C24   | 923  | PRO  | N-CD  | -11.70 | 1.31        | 1.47     |
| 5   | P8    | 148  | PRO  | N-CD  | -11.69 | 1.31        | 1.47     |
| 5   | P16   | 292  | GLU  | C-N   | -11.69 | 1.17        | 1.33     |
| 11  | A16   | 461  | VAL  | C-N   | -11.69 | 1.17        | 1.33     |
| 18  | B     | 524  | GLU  | C-N   | -11.69 | 1.19        | 1.33     |
| 18  | B8    | 1921 | PRO  | N-CD  | -11.69 | 1.31        | 1.47     |
| 5   | P     | 292  | GLU  | C-N   | -11.68 | 1.17        | 1.33     |
| 10  | C24   | 1162 | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 10  | C8    | 1162 | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 10  | C32   | 450  | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 10  | C32   | 923  | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 10  | C16   | 923  | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 11  | A16   | 788  | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 11  | A32   | 158  | PRO  | N-CD  | -11.68 | 1.31        | 1.47     |
| 5   | P     | 685  | PRO  | N-CD  | -11.67 | 1.31        | 1.47     |
| 10  | C     | 1726 | PRO  | N-CD  | -11.67 | 1.31        | 1.47     |
| 10  | C     | 923  | PRO  | N-CD  | -11.67 | 1.31        | 1.47     |
| 11  | A24   | 788  | PRO  | N-CD  | -11.66 | 1.31        | 1.47     |
| 10  | C24   | 400  | PRO  | N-CD  | -11.66 | 1.31        | 1.47     |
| 5   | P     | 155  | PRO  | N-CD  | -11.66 | 1.31        | 1.47     |
| 11  | A40   | 788  | PRO  | N-CD  | -11.65 | 1.31        | 1.47     |
| 5   | P16   | 148  | PRO  | N-CD  | -11.65 | 1.31        | 1.47     |
| 11  | A32   | 788  | PRO  | N-CD  | -11.64 | 1.31        | 1.47     |
| 10  | C8    | 400  | PRO  | N-CD  | -11.64 | 1.31        | 1.47     |
| 10  | C16   | 400  | PRO  | N-CD  | -11.64 | 1.31        | 1.47     |
| 14  | W     | 702  | PRO  | N-CD  | -11.64 | 1.31        | 1.47     |
| 12  | A     | 788  | PRO  | N-CD  | -11.63 | 1.31        | 1.47     |
| 12  | A     | 796  | ASP  | C-N   | -11.63 | 1.19        | 1.33     |
| 18  | B8    | 529  | PRO  | N-CD  | -11.63 | 1.31        | 1.47     |
| 2   | M     | 158  | PHE  | C-N   | 11.63  | 1.49        | 1.33     |
| 10  | C32   | 400  | PRO  | N-CD  | -11.62 | 1.31        | 1.47     |
| 12  | A48   | 461  | VAL  | C-N   | -11.62 | 1.17        | 1.33     |
| 11  | A24   | 796  | ASP  | C-N   | -11.62 | 1.19        | 1.33     |
| 10  | C     | 1162 | PRO  | N-CD  | -11.61 | 1.31        | 1.47     |
| 18  | B     | 1921 | PRO  | N-CD  | -11.61 | 1.31        | 1.47     |
| 12  | A48   | 788  | PRO  | N-CD  | -11.61 | 1.31        | 1.47     |
| 10  | C16   | 1162 | PRO  | N-CD  | -11.60 | 1.31        | 1.47     |
| 11  | A24   | 461  | VAL  | C-N   | -11.59 | 1.17        | 1.33     |
| 12  | A48   | 796  | ASP  | C-N   | -11.59 | 1.19        | 1.33     |
| 10  | C32   | 1726 | PRO  | N-CD  | -11.58 | 1.31        | 1.47     |
| 23  | J16   | 716  | ARG  | C-N   | -11.58 | 1.19        | 1.33     |
| 11  | A40   | 461  | VAL  | C-N   | -11.58 | 1.17        | 1.33     |
| 11  | A40   | 796  | ASP  | C-N   | -11.57 | 1.19        | 1.33     |
| 18  | B     | 504  | PRO  | N-CD  | -11.57 | 1.31        | 1.47     |
| 18  | B8    | 504  | PRO  | N-CD  | -11.57 | 1.31        | 1.47     |
| 18  | B8    | 1860 | PRO  | N-CD  | -11.57 | 1.31        | 1.47     |
| 2   | M16   | 158  | PHE  | C-N   | 11.56  | 1.49        | 1.33     |
| 23  | J8    | 716  | ARG  | C-N   | -11.56 | 1.19        | 1.33     |
| 10  | C24   | 1726 | PRO  | N-CD  | -11.55 | 1.31        | 1.47     |
| 10  | C16   | 1726 | PRO  | N-CD  | -11.55 | 1.31        | 1.47     |
| 12  | A     | 461  | VAL  | C-N   | -11.55 | 1.17        | 1.33     |
| 18  | B     | 529  | PRO  | N-CD  | -11.55 | 1.31        | 1.47     |
| 18  | B     | 568  | TYR  | C-N   | 11.54  | 1.47        | 1.34     |
| 11  | A16   | 796  | ASP  | C-N   | -11.54 | 1.19        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23  | J32   | 716  | ARG  | C-N   | -11.54 | 1.19        | 1.33     |
| 10  | C     | 400  | PRO  | N-CD  | -11.54 | 1.31        | 1.47     |
| 5   | P16   | 658  | PRO  | N-CD  | -11.54 | 1.31        | 1.47     |
| 1   | R8    | 1180 | PRO  | N-CD  | -11.53 | 1.31        | 1.47     |
| 1   | R16   | 1180 | PRO  | N-CD  | -11.53 | 1.31        | 1.47     |
| 11  | A32   | 796  | ASP  | C-N   | -11.53 | 1.19        | 1.33     |
| 10  | C32   | 1162 | PRO  | N-CD  | -11.53 | 1.31        | 1.47     |
| 2   | M8    | 761  | PRO  | N-CD  | -11.52 | 1.31        | 1.47     |
| 23  | J24   | 716  | ARG  | C-N   | -11.52 | 1.19        | 1.33     |
| 18  | B     | 1860 | PRO  | N-CD  | -11.52 | 1.31        | 1.47     |
| 2   | M8    | 158  | PHE  | C-N   | 11.51  | 1.48        | 1.33     |
| 10  | C     | 931  | PRO  | N-CD  | -11.51 | 1.31        | 1.47     |
| 11  | A32   | 461  | VAL  | C-N   | -11.50 | 1.17        | 1.33     |
| 1   | R     | 1180 | PRO  | N-CD  | -11.49 | 1.31        | 1.47     |
| 2   | M     | 761  | PRO  | N-CD  | -11.49 | 1.31        | 1.47     |
| 5   | P     | 658  | PRO  | N-CD  | -11.49 | 1.31        | 1.47     |
| 23  | J24   | 734  | PRO  | N-CD  | -11.49 | 1.31        | 1.47     |
| 18  | B8    | 568  | TYR  | C-N   | 11.49  | 1.47        | 1.34     |
| 10  | C8    | 1106 | PRO  | N-CD  | -11.48 | 1.31        | 1.47     |
| 18  | B8    | 1255 | PRO  | N-CD  | -11.48 | 1.31        | 1.47     |
| 2   | M16   | 524  | PRO  | N-CD  | -11.47 | 1.31        | 1.47     |
| 2   | M16   | 761  | PRO  | N-CD  | -11.47 | 1.31        | 1.47     |
| 5   | P8    | 658  | PRO  | N-CD  | -11.47 | 1.31        | 1.47     |
| 20  | E     | 423  | PRO  | N-CD  | -11.47 | 1.31        | 1.47     |
| 10  | C16   | 972  | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 10  | C     | 1106 | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 10  | C32   | 931  | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 10  | C32   | 1106 | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 10  | C16   | 931  | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 18  | B     | 1255 | PRO  | N-CD  | -11.45 | 1.31        | 1.47     |
| 10  | C     | 1661 | LEU  | C-N   | -11.45 | 1.17        | 1.33     |
| 10  | C16   | 1661 | LEU  | C-N   | -11.43 | 1.17        | 1.33     |
| 2   | M16   | 814  | PRO  | C-N   | 11.43  | 1.49        | 1.33     |
| 20  | E8    | 423  | PRO  | N-CD  | -11.43 | 1.31        | 1.47     |
| 2   | M     | 814  | PRO  | C-N   | 11.42  | 1.49        | 1.33     |
| 2   | M8    | 814  | PRO  | C-N   | 11.42  | 1.49        | 1.33     |
| 10  | C24   | 972  | PRO  | N-CD  | -11.42 | 1.31        | 1.47     |
| 10  | C32   | 425  | PRO  | N-CD  | -11.42 | 1.31        | 1.47     |
| 18  | B     | 1666 | PRO  | N-CD  | -11.42 | 1.31        | 1.47     |
| 10  | C8    | 931  | PRO  | N-CD  | -11.41 | 1.31        | 1.47     |
| 3   | N     | 161  | ALA  | C-N   | -11.40 | 1.17        | 1.33     |
| 10  | C24   | 931  | PRO  | N-CD  | -11.40 | 1.31        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 2   | M     | 524  | PRO  | N-CD  | -11.40 | 1.31        | 1.47     |
| 23  | J8    | 734  | PRO  | N-CD  | -11.40 | 1.31        | 1.47     |
| 23  | J16   | 734  | PRO  | N-CD  | -11.40 | 1.31        | 1.47     |
| 10  | C16   | 425  | PRO  | N-CD  | -11.39 | 1.31        | 1.47     |
| 1   | R16   | 1294 | PRO  | N-CD  | -11.39 | 1.31        | 1.47     |
| 23  | J32   | 734  | PRO  | N-CD  | -11.39 | 1.31        | 1.47     |
| 2   | M8    | 524  | PRO  | N-CD  | -11.38 | 1.31        | 1.47     |
| 10  | C     | 972  | PRO  | N-CD  | -11.38 | 1.31        | 1.47     |
| 14  | W     | 600  | PRO  | N-CD  | -11.37 | 1.31        | 1.47     |
| 10  | C24   | 425  | PRO  | N-CD  | -11.37 | 1.31        | 1.47     |
| 13  | V     | 876  | PRO  | N-CD  | -11.37 | 1.31        | 1.47     |
| 10  | C8    | 972  | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 21  | H16   | 325  | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 10  | C8    | 425  | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 18  | B8    | 1666 | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 10  | C32   | 1661 | LEU  | C-N   | -11.36 | 1.17        | 1.33     |
| 10  | C16   | 1106 | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 10  | C24   | 1106 | PRO  | N-CD  | -11.36 | 1.31        | 1.47     |
| 3   | N8    | 161  | ALA  | C-N   | -11.34 | 1.17        | 1.33     |
| 1   | R8    | 1294 | PRO  | N-CD  | -11.34 | 1.31        | 1.47     |
| 10  | C8    | 684  | PRO  | N-CD  | -11.34 | 1.31        | 1.47     |
| 10  | C8    | 1775 | VAL  | C-N   | 11.33  | 1.49        | 1.33     |
| 10  | C32   | 972  | PRO  | N-CD  | -11.32 | 1.31        | 1.47     |
| 10  | C     | 1775 | VAL  | C-N   | 11.32  | 1.49        | 1.33     |
| 10  | C24   | 1775 | VAL  | C-N   | 11.32  | 1.49        | 1.33     |
| 10  | C     | 425  | PRO  | N-CD  | -11.32 | 1.31        | 1.47     |
| 10  | C24   | 1661 | LEU  | C-N   | -11.30 | 1.17        | 1.33     |
| 21  | H     | 325  | PRO  | N-CD  | -11.30 | 1.31        | 1.47     |
| 21  | H24   | 325  | PRO  | N-CD  | -11.30 | 1.31        | 1.47     |
| 21  | H8    | 325  | PRO  | N-CD  | -11.30 | 1.31        | 1.47     |
| 22  | I16   | 370  | PRO  | C-N   | 11.30  | 1.49        | 1.33     |
| 10  | C32   | 1775 | VAL  | C-N   | 11.29  | 1.49        | 1.33     |
| 10  | C24   | 1619 | PRO  | N-CD  | -11.29 | 1.31        | 1.47     |
| 1   | R     | 1294 | PRO  | N-CD  | -11.28 | 1.31        | 1.47     |
| 10  | C8    | 51   | PRO  | N-CD  | -11.28 | 1.31        | 1.47     |
| 5   | P     | 150  | PRO  | N-CD  | -11.27 | 1.31        | 1.47     |
| 22  | I24   | 370  | PRO  | C-N   | 11.27  | 1.49        | 1.33     |
| 9   | K8    | 650  | THR  | C-N   | -11.27 | 1.19        | 1.33     |
| 7   | Q     | 58   | PRO  | N-CD  | -11.26 | 1.31        | 1.47     |
| 5   | P16   | 392  | PRO  | N-CD  | -11.26 | 1.31        | 1.47     |
| 5   | P8    | 392  | PRO  | N-CD  | -11.25 | 1.32        | 1.47     |
| 10  | C16   | 1775 | VAL  | C-N   | 11.24  | 1.49        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 5   | P     | 392  | PRO  | N-CD  | -11.24 | 1.32        | 1.47     |
| 3   | N16   | 161  | ALA  | C-N   | -11.23 | 1.17        | 1.33     |
| 5   | P16   | 150  | PRO  | N-CD  | -11.23 | 1.32        | 1.47     |
| 22  | I8    | 370  | PRO  | C-N   | 11.23  | 1.49        | 1.33     |
| 18  | B8    | 192  | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 5   | P8    | 150  | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 10  | C8    | 1619 | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 10  | C32   | 1619 | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 7   | Q8    | 58   | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 14  | W     | 594  | PRO  | N-CD  | -11.22 | 1.32        | 1.47     |
| 10  | C     | 561  | ASN  | C-N   | -11.21 | 1.19        | 1.33     |
| 18  | B     | 1903 | THR  | C-N   | -11.21 | 1.19        | 1.33     |
| 10  | C32   | 561  | ASN  | C-N   | -11.21 | 1.19        | 1.33     |
| 10  | C8    | 620  | PRO  | N-CD  | -11.21 | 1.32        | 1.47     |
| 22  | I     | 370  | PRO  | C-N   | 11.21  | 1.49        | 1.33     |
| 20  | E     | 420  | LEU  | C-N   | 11.21  | 1.49        | 1.33     |
| 10  | C24   | 1070 | PRO  | N-CD  | -11.20 | 1.32        | 1.47     |
| 18  | B8    | 1903 | THR  | C-N   | -11.21 | 1.19        | 1.33     |
| 20  | E8    | 420  | LEU  | C-N   | 11.21  | 1.49        | 1.33     |
| 20  | E     | 344  | PRO  | N-CD  | -11.20 | 1.32        | 1.47     |
| 7   | Q16   | 58   | PRO  | N-CD  | -11.20 | 1.32        | 1.47     |
| 10  | C     | 684  | PRO  | N-CD  | -11.19 | 1.32        | 1.47     |
| 18  | B     | 192  | PRO  | N-CD  | -11.19 | 1.32        | 1.47     |
| 10  | C32   | 684  | PRO  | N-CD  | -11.18 | 1.32        | 1.47     |
| 18  | B     | 1594 | PRO  | N-CD  | -11.18 | 1.32        | 1.47     |
| 20  | E8    | 344  | PRO  | N-CD  | -11.18 | 1.32        | 1.47     |
| 18  | B8    | 1291 | LEU  | C-N   | 11.18  | 1.48        | 1.33     |
| 10  | C     | 620  | PRO  | N-CD  | -11.16 | 1.32        | 1.47     |
| 9   | K     | 1235 | GLU  | C-N   | 11.16  | 1.51        | 1.33     |
| 10  | C16   | 1665 | THR  | C-N   | 11.16  | 1.48        | 1.33     |
| 10  | C     | 1619 | PRO  | N-CD  | -11.16 | 1.32        | 1.47     |
| 18  | B8    | 1594 | PRO  | N-CD  | -11.16 | 1.32        | 1.47     |
| 9   | K8    | 1235 | GLU  | C-N   | 11.16  | 1.51        | 1.33     |
| 9   | K     | 650  | THR  | C-N   | -11.15 | 1.20        | 1.33     |
| 10  | C24   | 684  | PRO  | N-CD  | -11.15 | 1.32        | 1.47     |
| 18  | B     | 1113 | PRO  | N-CD  | -11.15 | 1.32        | 1.47     |
| 10  | C16   | 561  | ASN  | C-N   | -11.15 | 1.19        | 1.33     |
| 10  | C16   | 620  | PRO  | N-CD  | -11.14 | 1.32        | 1.47     |
| 18  | B     | 1291 | LEU  | C-N   | 11.14  | 1.48        | 1.33     |
| 18  | B     | 1807 | PRO  | N-CD  | -11.14 | 1.32        | 1.47     |
| 10  | C16   | 51   | PRO  | N-CD  | -11.14 | 1.32        | 1.47     |
| 1   | R8    | 1189 | PRO  | N-CD  | -11.13 | 1.32        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 18  | B8    | 1807 | PRO  | N-CD  | -11.13 | 1.32        | 1.47     |
| 10  | C32   | 51   | PRO  | N-CD  | -11.13 | 1.32        | 1.47     |
| 18  | B8    | 1669 | PRO  | N-CD  | -11.13 | 1.32        | 1.47     |
| 10  | C24   | 561  | ASN  | C-N   | -11.12 | 1.19        | 1.33     |
| 10  | C32   | 620  | PRO  | N-CD  | -11.12 | 1.32        | 1.47     |
| 10  | C16   | 1619 | PRO  | N-CD  | -11.12 | 1.32        | 1.47     |
| 3   | N     | 2    | PRO  | N-CD  | -11.12 | 1.32        | 1.47     |
| 10  | C24   | 620  | PRO  | N-CD  | -11.12 | 1.32        | 1.47     |
| 19  | 4     | 185  | GLY  | C-N   | -11.12 | 1.17        | 1.33     |
| 17  | F     | 70   | PRO  | N-CD  | -11.12 | 1.32        | 1.47     |
| 17  | F8    | 70   | PRO  | N-CD  | -11.11 | 1.32        | 1.47     |
| 18  | B8    | 157  | PRO  | C-N   | 11.11  | 1.48        | 1.33     |
| 10  | C32   | 1665 | THR  | C-N   | 11.11  | 1.48        | 1.33     |
| 10  | C16   | 648  | ALA  | C-N   | 11.11  | 1.49        | 1.34     |
| 10  | C     | 51   | PRO  | N-CD  | -11.11 | 1.32        | 1.47     |
| 10  | C16   | 604  | PRO  | N-CD  | -11.10 | 1.32        | 1.47     |
| 10  | C16   | 684  | PRO  | N-CD  | -11.10 | 1.32        | 1.47     |
| 3   | N8    | 2    | PRO  | N-CD  | -11.09 | 1.32        | 1.47     |
| 10  | C8    | 648  | ALA  | C-N   | 11.09  | 1.49        | 1.34     |
| 10  | C24   | 648  | ALA  | C-N   | 11.09  | 1.49        | 1.34     |
| 10  | C8    | 604  | PRO  | N-CD  | -11.09 | 1.32        | 1.47     |
| 17  | F16   | 70   | PRO  | N-CD  | -11.09 | 1.32        | 1.47     |
| 10  | C32   | 719  | PRO  | N-CD  | -11.09 | 1.32        | 1.47     |
| 10  | C     | 648  | ALA  | C-N   | 11.08  | 1.49        | 1.34     |
| 10  | C32   | 604  | PRO  | N-CD  | -11.08 | 1.32        | 1.47     |
| 1   | R     | 1189 | PRO  | N-CD  | -11.08 | 1.32        | 1.47     |
| 3   | N16   | 2    | PRO  | N-CD  | -11.08 | 1.32        | 1.47     |
| 10  | C     | 604  | PRO  | N-CD  | -11.08 | 1.32        | 1.47     |
| 10  | C32   | 1070 | PRO  | N-CD  | -11.07 | 1.32        | 1.47     |
| 17  | F24   | 70   | PRO  | N-CD  | -11.07 | 1.32        | 1.47     |
| 12  | A     | 791  | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 10  | C24   | 51   | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 10  | C24   | 604  | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 18  | B     | 990  | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 19  | 48    | 185  | GLY  | C-N   | -11.06 | 1.17        | 1.33     |
| 1   | R     | 1207 | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 10  | C     | 1070 | PRO  | N-CD  | -11.06 | 1.32        | 1.47     |
| 10  | C16   | 719  | PRO  | N-CD  | -11.05 | 1.32        | 1.47     |
| 18  | B     | 157  | PRO  | C-N   | 11.05  | 1.48        | 1.33     |
| 18  | B8    | 1113 | PRO  | N-CD  | -11.05 | 1.32        | 1.47     |
| 10  | C16   | 1070 | PRO  | N-CD  | -11.05 | 1.32        | 1.47     |
| 10  | C32   | 648  | ALA  | C-N   | 11.05  | 1.49        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C8    | 562  | PRO  | N-CD  | -11.04 | 1.32        | 1.47     |
| 9   | K     | 713  | ASN  | C-N   | -11.03 | 1.18        | 1.33     |
| 18  | B8    | 342  | PRO  | N-CD  | -11.04 | 1.32        | 1.47     |
| 18  | B     | 1669 | PRO  | N-CD  | -11.03 | 1.32        | 1.47     |
| 11  | A24   | 791  | PRO  | N-CD  | -11.03 | 1.32        | 1.47     |
| 10  | C8    | 561  | ASN  | C-N   | -11.03 | 1.19        | 1.33     |
| 18  | B8    | 1258 | PRO  | N-CD  | -11.01 | 1.32        | 1.47     |
| 22  | I24   | 207  | PRO  | N-CD  | -11.01 | 1.32        | 1.47     |
| 1   | R16   | 1189 | PRO  | N-CD  | -11.01 | 1.32        | 1.47     |
| 10  | C24   | 719  | PRO  | N-CD  | -11.01 | 1.32        | 1.47     |
| 1   | R8    | 1207 | PRO  | N-CD  | -11.01 | 1.32        | 1.47     |
| 10  | C     | 1665 | THR  | C-N   | 11.01  | 1.48        | 1.33     |
| 20  | E     | 305  | GLU  | C-N   | -11.01 | 1.19        | 1.33     |
| 10  | C     | 1357 | LEU  | C-N   | -11.00 | 1.18        | 1.33     |
| 10  | C8    | 1070 | PRO  | N-CD  | -11.00 | 1.32        | 1.47     |
| 22  | I8    | 207  | PRO  | N-CD  | -11.00 | 1.32        | 1.47     |
| 9   | K     | 1277 | ALA  | C-N   | 11.00  | 1.49        | 1.33     |
| 20  | E8    | 305  | GLU  | C-N   | -11.00 | 1.19        | 1.33     |
| 18  | B     | 342  | PRO  | N-CD  | -10.99 | 1.32        | 1.47     |
| 18  | B8    | 678  | PRO  | N-CD  | -10.99 | 1.32        | 1.47     |
| 10  | C8    | 1357 | LEU  | C-N   | -10.98 | 1.18        | 1.33     |
| 1   | R16   | 1207 | PRO  | N-CD  | -10.98 | 1.32        | 1.47     |
| 10  | C     | 719  | PRO  | N-CD  | -10.97 | 1.32        | 1.47     |
| 9   | K8    | 713  | ASN  | C-N   | -10.97 | 1.18        | 1.33     |
| 9   | K8    | 1277 | ALA  | C-N   | 10.97  | 1.49        | 1.33     |
| 10  | C24   | 1665 | THR  | C-N   | 10.97  | 1.47        | 1.33     |
| 3   | N8    | 302  | PRO  | N-CD  | -10.97 | 1.32        | 1.47     |
| 18  | B8    | 990  | PRO  | N-CD  | -10.96 | 1.32        | 1.47     |
| 22  | I16   | 207  | PRO  | N-CD  | -10.96 | 1.32        | 1.47     |
| 10  | C32   | 562  | PRO  | N-CD  | -10.96 | 1.32        | 1.47     |
| 5   | P8    | 2    | PRO  | N-CD  | -10.95 | 1.32        | 1.47     |
| 10  | C16   | 562  | PRO  | N-CD  | -10.95 | 1.32        | 1.47     |
| 11  | A24   | 560  | MET  | C-N   | -10.95 | 1.17        | 1.33     |
| 22  | I     | 207  | PRO  | N-CD  | -10.95 | 1.32        | 1.47     |
| 12  | A48   | 791  | PRO  | N-CD  | -10.95 | 1.32        | 1.47     |
| 18  | B8    | 519  | HIS  | C-N   | -10.94 | 1.24        | 1.33     |
| 18  | B     | 1258 | PRO  | N-CD  | -10.94 | 1.32        | 1.47     |
| 10  | C24   | 562  | PRO  | N-CD  | -10.93 | 1.32        | 1.47     |
| 10  | C32   | 1357 | LEU  | C-N   | -10.93 | 1.18        | 1.33     |
| 11  | A32   | 560  | MET  | C-N   | -10.93 | 1.17        | 1.33     |
| 18  | B     | 678  | PRO  | N-CD  | -10.93 | 1.32        | 1.47     |
| 12  | A     | 560  | MET  | C-N   | -10.93 | 1.17        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 11  | A40   | 791  | PRO  | N-CD  | -10.92 | 1.32        | 1.47     |
| 10  | C16   | 1357 | LEU  | C-N   | -10.91 | 1.18        | 1.33     |
| 3   | N     | 302  | PRO  | N-CD  | -10.90 | 1.32        | 1.47     |
| 10  | C     | 562  | PRO  | N-CD  | -10.90 | 1.32        | 1.47     |
| 5   | P     | 2    | PRO  | N-CD  | -10.90 | 1.32        | 1.47     |
| 10  | C24   | 1357 | LEU  | C-N   | -10.90 | 1.18        | 1.33     |
| 11  | A32   | 791  | PRO  | N-CD  | -10.90 | 1.32        | 1.47     |
| 9   | K     | 1181 | ASP  | C-N   | -10.89 | 1.18        | 1.33     |
| 11  | A16   | 791  | PRO  | N-CD  | -10.89 | 1.32        | 1.47     |
| 10  | C32   | 1243 | PRO  | N-CD  | -10.89 | 1.32        | 1.47     |
| 11  | A16   | 560  | MET  | C-N   | -10.88 | 1.17        | 1.33     |
| 18  | B     | 519  | HIS  | C-N   | -10.88 | 1.24        | 1.33     |
| 22  | I16   | 295  | SER  | C-N   | 10.88  | 1.45        | 1.33     |
| 10  | C     | 1243 | PRO  | N-CD  | -10.88 | 1.32        | 1.47     |
| 11  | A40   | 560  | MET  | C-N   | -10.87 | 1.17        | 1.33     |
| 20  | E     | 347  | PRO  | N-CD  | -10.85 | 1.32        | 1.47     |
| 22  | I24   | 295  | SER  | C-N   | 10.85  | 1.45        | 1.33     |
| 9   | K     | 677  | GLU  | C-N   | -10.83 | 1.19        | 1.33     |
| 10  | C16   | 1243 | PRO  | N-CD  | -10.83 | 1.32        | 1.47     |
| 10  | C     | 38   | PRO  | N-CD  | -10.83 | 1.32        | 1.47     |
| 5   | P16   | 2    | PRO  | N-CD  | -10.82 | 1.32        | 1.47     |
| 12  | A48   | 560  | MET  | C-N   | -10.82 | 1.17        | 1.33     |
| 9   | K8    | 677  | GLU  | C-N   | -10.82 | 1.19        | 1.33     |
| 9   | K8    | 1181 | ASP  | C-N   | -10.81 | 1.18        | 1.33     |
| 3   | N16   | 302  | PRO  | N-CD  | -10.81 | 1.32        | 1.47     |
| 22  | I16   | 255  | PRO  | N-CD  | -10.81 | 1.32        | 1.47     |
| 20  | E8    | 347  | PRO  | N-CD  | -10.80 | 1.32        | 1.47     |
| 13  | V     | 832  | LEU  | C-N   | -10.80 | 1.11        | 1.33     |
| 10  | C24   | 1243 | PRO  | N-CD  | -10.79 | 1.32        | 1.47     |
| 10  | C24   | 528  | LEU  | C-N   | 10.78  | 1.50        | 1.33     |
| 10  | C8    | 1243 | PRO  | N-CD  | -10.78 | 1.32        | 1.47     |
| 10  | C24   | 189  | PRO  | N-CD  | -10.78 | 1.32        | 1.47     |
| 19  | 48    | 447  | PRO  | N-CD  | -10.78 | 1.32        | 1.47     |
| 22  | I8    | 295  | SER  | C-N   | 10.77  | 1.45        | 1.33     |
| 10  | C32   | 189  | PRO  | N-CD  | -10.77 | 1.32        | 1.47     |
| 22  | I8    | 204  | PRO  | N-CD  | -10.77 | 1.32        | 1.47     |
| 19  | 4     | 447  | PRO  | N-CD  | -10.77 | 1.32        | 1.47     |
| 10  | C16   | 189  | PRO  | N-CD  | -10.76 | 1.32        | 1.47     |
| 13  | V     | 834  | PRO  | N-CD  | -10.76 | 1.32        | 1.47     |
| 10  | C32   | 38   | PRO  | N-CD  | -10.76 | 1.32        | 1.47     |
| 10  | C24   | 570  | PRO  | N-CD  | -10.76 | 1.32        | 1.47     |
| 22  | I8    | 255  | PRO  | N-CD  | -10.76 | 1.32        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C8    | 38   | PRO  | N-CD  | -10.74 | 1.32        | 1.47     |
| 22  | I     | 295  | SER  | C-N   | 10.74  | 1.45        | 1.33     |
| 10  | C24   | 38   | PRO  | N-CD  | -10.74 | 1.32        | 1.47     |
| 10  | C     | 570  | PRO  | N-CD  | -10.74 | 1.32        | 1.47     |
| 10  | C8    | 570  | PRO  | N-CD  | -10.74 | 1.32        | 1.47     |
| 22  | I24   | 255  | PRO  | N-CD  | -10.74 | 1.32        | 1.47     |
| 10  | C32   | 1168 | PRO  | N-CD  | -10.73 | 1.32        | 1.47     |
| 1   | R16   | 1380 | LYS  | C-N   | 10.73  | 1.48        | 1.33     |
| 22  | I     | 204  | PRO  | N-CD  | -10.73 | 1.32        | 1.47     |
| 10  | C16   | 528  | LEU  | C-N   | 10.72  | 1.49        | 1.33     |
| 10  | C8    | 189  | PRO  | N-CD  | -10.72 | 1.32        | 1.47     |
| 10  | C32   | 570  | PRO  | N-CD  | -10.72 | 1.32        | 1.47     |
| 9   | K8    | 726  | GLU  | C-N   | 10.71  | 1.48        | 1.33     |
| 10  | C24   | 1168 | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 10  | C16   | 570  | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 22  | I     | 255  | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 22  | I16   | 204  | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 10  | C32   | 528  | LEU  | C-N   | 10.71  | 1.49        | 1.33     |
| 9   | K     | 1237 | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 10  | C16   | 38   | PRO  | N-CD  | -10.71 | 1.32        | 1.47     |
| 18  | B     | 346  | GLU  | C-N   | 10.70  | 1.46        | 1.33     |
| 10  | C     | 1168 | PRO  | N-CD  | -10.70 | 1.32        | 1.47     |
| 22  | I24   | 204  | PRO  | N-CD  | -10.69 | 1.32        | 1.47     |
| 9   | K     | 726  | GLU  | C-N   | 10.69  | 1.48        | 1.33     |
| 3   | N16   | 175  | PRO  | N-CD  | -10.69 | 1.32        | 1.47     |
| 18  | B8    | 346  | GLU  | C-N   | 10.68  | 1.46        | 1.33     |
| 10  | C     | 1627 | GLY  | C-N   | -10.68 | 1.17        | 1.33     |
| 22  | I     | 147  | SER  | C-N   | -10.68 | 1.20        | 1.33     |
| 1   | R     | 1380 | LYS  | C-N   | 10.67  | 1.48        | 1.33     |
| 10  | C8    | 528  | LEU  | C-N   | 10.66  | 1.49        | 1.33     |
| 9   | K     | 1283 | PRO  | N-CD  | -10.66 | 1.32        | 1.47     |
| 10  | C8    | 1168 | PRO  | N-CD  | -10.65 | 1.32        | 1.47     |
| 9   | K8    | 1237 | PRO  | N-CD  | -10.65 | 1.32        | 1.47     |
| 10  | C     | 189  | PRO  | N-CD  | -10.65 | 1.32        | 1.47     |
| 22  | I24   | 147  | SER  | C-N   | -10.65 | 1.20        | 1.33     |
| 10  | C     | 528  | LEU  | C-N   | 10.64  | 1.49        | 1.33     |
| 21  | H24   | 294  | PRO  | N-CD  | -10.64 | 1.32        | 1.47     |
| 9   | K8    | 1283 | PRO  | N-CD  | -10.63 | 1.32        | 1.47     |
| 10  | C24   | 1627 | GLY  | C-N   | -10.63 | 1.17        | 1.33     |
| 19  | 48    | 51   | PRO  | N-CD  | -10.63 | 1.32        | 1.47     |
| 9   | K     | 1254 | PHE  | C-N   | 10.62  | 1.48        | 1.33     |
| 19  | 4     | 51   | PRO  | N-CD  | -10.61 | 1.32        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 11  | A40   | 846  | HIS  | C-N   | -10.61 | 1.18        | 1.33     |
| 9   | K8    | 1254 | PHE  | C-N   | 10.61  | 1.48        | 1.33     |
| 10  | C32   | 1627 | GLY  | C-N   | -10.60 | 1.17        | 1.33     |
| 11  | A24   | 846  | HIS  | C-N   | -10.60 | 1.18        | 1.33     |
| 9   | K     | 787  | PRO  | N-CD  | -10.60 | 1.32        | 1.47     |
| 22  | I8    | 147  | SER  | C-N   | -10.60 | 1.20        | 1.33     |
| 7   | Q     | 361  | PRO  | N-CD  | -10.59 | 1.32        | 1.47     |
| 7   | Q8    | 361  | PRO  | N-CD  | -10.59 | 1.32        | 1.47     |
| 10  | C16   | 1168 | PRO  | N-CD  | -10.59 | 1.32        | 1.47     |
| 23  | J8    | 725  | SER  | C-N   | 10.59  | 1.49        | 1.33     |
| 11  | A16   | 846  | HIS  | C-N   | -10.58 | 1.18        | 1.33     |
| 19  | 48    | 189  | LEU  | C-N   | -10.58 | 1.18        | 1.33     |
| 11  | A32   | 846  | HIS  | C-N   | -10.58 | 1.18        | 1.33     |
| 5   | P     | 14   | VAL  | C-N   | -10.57 | 1.20        | 1.34     |
| 1   | R8    | 1380 | LYS  | C-N   | 10.57  | 1.48        | 1.33     |
| 7   | Q16   | 361  | PRO  | N-CD  | -10.57 | 1.32        | 1.47     |
| 9   | K8    | 787  | PRO  | N-CD  | -10.57 | 1.32        | 1.47     |
| 23  | J24   | 725  | SER  | C-N   | 10.57  | 1.49        | 1.33     |
| 20  | E     | 348  | PRO  | N-CD  | -10.56 | 1.32        | 1.47     |
| 10  | C8    | 1593 | TRP  | C-N   | 10.56  | 1.45        | 1.34     |
| 5   | P16   | 14   | VAL  | C-N   | -10.56 | 1.20        | 1.34     |
| 21  | H8    | 294  | PRO  | N-CD  | -10.56 | 1.32        | 1.47     |
| 14  | W     | 615  | GLU  | C-N   | -10.55 | 1.20        | 1.33     |
| 21  | H16   | 294  | PRO  | N-CD  | -10.56 | 1.32        | 1.47     |
| 22  | I16   | 147  | SER  | C-N   | -10.55 | 1.20        | 1.33     |
| 20  | E8    | 348  | PRO  | N-CD  | -10.55 | 1.32        | 1.47     |
| 22  | I24   | 151  | GLU  | C-N   | -10.55 | 1.21        | 1.34     |
| 12  | A48   | 846  | HIS  | C-N   | -10.55 | 1.18        | 1.33     |
| 19  | 4     | 189  | LEU  | C-N   | -10.55 | 1.19        | 1.33     |
| 10  | C16   | 1627 | GLY  | C-N   | -10.55 | 1.17        | 1.33     |
| 10  | C     | 1593 | TRP  | C-N   | 10.54  | 1.45        | 1.34     |
| 21  | H     | 294  | PRO  | N-CD  | -10.54 | 1.32        | 1.47     |
| 12  | A     | 846  | HIS  | C-N   | -10.54 | 1.18        | 1.33     |
| 20  | E8    | 429  | PRO  | N-CD  | -10.54 | 1.33        | 1.47     |
| 3   | N8    | 175  | PRO  | N-CD  | -10.53 | 1.33        | 1.47     |
| 5   | P8    | 14   | VAL  | C-N   | -10.53 | 1.20        | 1.34     |
| 10  | C24   | 183  | PRO  | N-CD  | -10.53 | 1.33        | 1.47     |
| 22  | I16   | 151  | GLU  | C-N   | -10.53 | 1.21        | 1.34     |
| 10  | C16   | 1611 | MET  | C-N   | 10.52  | 1.48        | 1.34     |
| 23  | J16   | 725  | SER  | C-N   | 10.51  | 1.48        | 1.33     |
| 12  | A48   | 340  | PRO  | N-CD  | -10.51 | 1.33        | 1.47     |
| 19  | 4     | 53   | SER  | C-N   | -10.51 | 1.19        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23  | J32   | 725  | SER  | C-N   | 10.50  | 1.48        | 1.33     |
| 3   | N     | 175  | PRO  | N-CD  | -10.50 | 1.33        | 1.47     |
| 10  | C8    | 1627 | GLY  | C-N   | -10.50 | 1.17        | 1.33     |
| 19  | 48    | 53   | SER  | C-N   | -10.50 | 1.19        | 1.33     |
| 10  | C32   | 183  | PRO  | N-CD  | -10.49 | 1.33        | 1.47     |
| 18  | B8    | 1849 | GLY  | C-N   | 10.49  | 1.46        | 1.33     |
| 10  | C8    | 183  | PRO  | N-CD  | -10.49 | 1.33        | 1.47     |
| 22  | I8    | 151  | GLU  | C-N   | -10.49 | 1.21        | 1.34     |
| 10  | C8    | 1611 | MET  | C-N   | 10.49  | 1.48        | 1.34     |
| 20  | E     | 429  | PRO  | N-CD  | -10.49 | 1.33        | 1.47     |
| 10  | C16   | 183  | PRO  | N-CD  | -10.48 | 1.33        | 1.47     |
| 11  | A24   | 340  | PRO  | N-CD  | -10.48 | 1.33        | 1.47     |
| 22  | I     | 151  | GLU  | C-N   | -10.48 | 1.21        | 1.34     |
| 9   | K8    | 1118 | PRO  | N-CD  | -10.47 | 1.33        | 1.47     |
| 3   | N16   | 220  | PRO  | N-CD  | -10.47 | 1.33        | 1.47     |
| 11  | A16   | 340  | PRO  | N-CD  | -10.47 | 1.33        | 1.47     |
| 10  | C24   | 1593 | TRP  | C-N   | 10.47  | 1.45        | 1.34     |
| 10  | C     | 183  | PRO  | N-CD  | -10.47 | 1.33        | 1.47     |
| 10  | C8    | 1500 | MET  | C-N   | 10.47  | 1.48        | 1.33     |
| 18  | B     | 293  | PRO  | N-CD  | -10.47 | 1.33        | 1.47     |
| 9   | K     | 1118 | PRO  | N-CD  | -10.46 | 1.33        | 1.47     |
| 9   | K8    | 725  | SER  | C-N   | 10.46  | 1.48        | 1.33     |
| 12  | A     | 340  | PRO  | N-CD  | -10.46 | 1.33        | 1.47     |
| 10  | C     | 1611 | MET  | C-N   | 10.46  | 1.48        | 1.34     |
| 10  | C32   | 1732 | LYS  | C-N   | -10.46 | 1.20        | 1.33     |
| 23  | J8    | 737  | TRP  | C-N   | 10.45  | 1.49        | 1.33     |
| 10  | C32   | 1611 | MET  | C-N   | 10.44  | 1.48        | 1.34     |
| 11  | A24   | 99   | THR  | C-N   | 10.44  | 1.48        | 1.33     |
| 11  | A32   | 340  | PRO  | N-CD  | -10.44 | 1.33        | 1.47     |
| 12  | A48   | 99   | THR  | C-N   | 10.44  | 1.48        | 1.33     |
| 10  | C32   | 1593 | TRP  | C-N   | 10.43  | 1.45        | 1.34     |
| 3   | N     | 220  | PRO  | N-CD  | -10.43 | 1.33        | 1.47     |
| 9   | K     | 725  | SER  | C-N   | 10.43  | 1.48        | 1.33     |
| 18  | B     | 1948 | PRO  | N-CD  | -10.43 | 1.33        | 1.47     |
| 10  | C24   | 1732 | LYS  | C-N   | -10.42 | 1.20        | 1.33     |
| 10  | C32   | 1500 | MET  | C-N   | 10.42  | 1.48        | 1.33     |
| 11  | A40   | 340  | PRO  | N-CD  | -10.41 | 1.33        | 1.47     |
| 3   | N8    | 220  | PRO  | N-CD  | -10.41 | 1.33        | 1.47     |
| 10  | C24   | 1611 | MET  | C-N   | 10.41  | 1.48        | 1.34     |
| 18  | B8    | 293  | PRO  | N-CD  | -10.41 | 1.33        | 1.47     |
| 18  | B     | 1849 | GLY  | C-N   | 10.40  | 1.46        | 1.33     |
| 18  | B8    | 1948 | PRO  | N-CD  | -10.40 | 1.33        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23  | J24   | 737  | TRP  | C-N   | 10.40  | 1.49        | 1.33     |
| 10  | C16   | 1500 | MET  | C-N   | 10.40  | 1.48        | 1.33     |
| 10  | C16   | 1659 | ASP  | C-N   | -10.40 | 1.20        | 1.33     |
| 23  | J16   | 737  | TRP  | C-N   | 10.40  | 1.49        | 1.33     |
| 10  | C     | 1500 | MET  | C-N   | 10.38  | 1.48        | 1.33     |
| 10  | C16   | 1593 | TRP  | C-N   | 10.38  | 1.45        | 1.34     |
| 10  | C     | 1659 | ASP  | C-N   | -10.38 | 1.20        | 1.33     |
| 10  | C16   | 1732 | LYS  | C-N   | -10.37 | 1.20        | 1.33     |
| 23  | J32   | 737  | TRP  | C-N   | 10.37  | 1.49        | 1.33     |
| 10  | C8    | 1732 | LYS  | C-N   | -10.36 | 1.20        | 1.33     |
| 11  | A40   | 99   | THR  | C-N   | 10.36  | 1.48        | 1.33     |
| 12  | A     | 99   | THR  | C-N   | 10.36  | 1.48        | 1.33     |
| 18  | B8    | 4    | PRO  | N-CD  | -10.36 | 1.33        | 1.47     |
| 10  | C24   | 1500 | MET  | C-N   | 10.35  | 1.48        | 1.33     |
| 16  | A8    | 99   | THR  | C-N   | 10.35  | 1.48        | 1.33     |
| 10  | C     | 1732 | LYS  | C-N   | -10.34 | 1.20        | 1.33     |
| 18  | B     | 1397 | PRO  | N-CD  | -10.34 | 1.33        | 1.47     |
| 14  | W     | 708  | PRO  | N-CD  | -10.32 | 1.33        | 1.47     |
| 18  | B     | 4    | PRO  | N-CD  | -10.31 | 1.33        | 1.47     |
| 10  | C32   | 449  | GLU  | C-N   | 10.28  | 1.47        | 1.34     |
| 10  | C32   | 1659 | ASP  | C-N   | -10.28 | 1.20        | 1.33     |
| 18  | B     | 1138 | PRO  | N-CD  | -10.28 | 1.33        | 1.47     |
| 18  | B     | 1717 | MET  | C-N   | -10.28 | 1.20        | 1.33     |
| 18  | B8    | 1717 | MET  | C-N   | -10.27 | 1.20        | 1.33     |
| 10  | C24   | 1292 | SER  | C-N   | -10.27 | 1.20        | 1.33     |
| 18  | B8    | 1138 | PRO  | N-CD  | -10.26 | 1.33        | 1.47     |
| 10  | C8    | 680  | ALA  | C-N   | 10.26  | 1.47        | 1.33     |
| 11  | A16   | 57   | PRO  | N-CD  | -10.26 | 1.33        | 1.47     |
| 18  | B8    | 1397 | PRO  | N-CD  | -10.25 | 1.33        | 1.47     |
| 10  | C     | 907  | PRO  | N-CD  | -10.25 | 1.33        | 1.47     |
| 10  | C32   | 907  | PRO  | N-CD  | -10.22 | 1.33        | 1.47     |
| 11  | A40   | 57   | PRO  | N-CD  | -10.22 | 1.33        | 1.47     |
| 10  | C16   | 449  | GLU  | C-N   | 10.21  | 1.47        | 1.34     |
| 10  | C16   | 1292 | SER  | C-N   | -10.22 | 1.20        | 1.33     |
| 10  | C24   | 1659 | ASP  | C-N   | -10.21 | 1.20        | 1.33     |
| 11  | A24   | 57   | PRO  | N-CD  | -10.20 | 1.33        | 1.47     |
| 11  | A32   | 57   | PRO  | N-CD  | -10.19 | 1.33        | 1.47     |
| 10  | C     | 330  | GLY  | C-N   | 10.19  | 1.46        | 1.33     |
| 10  | C8    | 907  | PRO  | N-CD  | -10.19 | 1.33        | 1.47     |
| 10  | C24   | 907  | PRO  | N-CD  | -10.18 | 1.33        | 1.47     |
| 18  | B8    | 159  | GLU  | C-N   | 10.18  | 1.46        | 1.33     |
| 10  | C24   | 330  | GLY  | C-N   | 10.18  | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C32   | 330  | GLY  | C-N   | 10.18  | 1.46        | 1.33     |
| 10  | C16   | 330  | GLY  | C-N   | 10.17  | 1.46        | 1.33     |
| 10  | C24   | 449  | GLU  | C-N   | 10.17  | 1.47        | 1.34     |
| 10  | C8    | 23   | PRO  | N-CD  | -10.17 | 1.33        | 1.47     |
| 1   | R16   | 1293 | CYS  | C-N   | 10.17  | 1.50        | 1.34     |
| 19  | 4     | 91   | PRO  | N-CD  | -10.17 | 1.33        | 1.47     |
| 10  | C32   | 23   | PRO  | N-CD  | -10.17 | 1.33        | 1.47     |
| 10  | C8    | 1292 | SER  | C-N   | -10.16 | 1.20        | 1.33     |
| 1   | R8    | 1293 | CYS  | C-N   | 10.16  | 1.50        | 1.34     |
| 18  | B     | 159  | GLU  | C-N   | 10.16  | 1.46        | 1.33     |
| 1   | R     | 1224 | VAL  | C-N   | -10.16 | 1.20        | 1.33     |
| 10  | C32   | 1292 | SER  | C-N   | -10.16 | 1.20        | 1.33     |
| 10  | C16   | 23   | PRO  | N-CD  | -10.15 | 1.33        | 1.47     |
| 13  | V     | 888  | PRO  | N-CD  | -10.15 | 1.33        | 1.47     |
| 1   | R     | 1293 | CYS  | C-N   | 10.14  | 1.50        | 1.34     |
| 1   | R8    | 1224 | VAL  | C-N   | -10.14 | 1.20        | 1.33     |
| 10  | C16   | 680  | ALA  | C-N   | 10.14  | 1.47        | 1.33     |
| 10  | C8    | 1802 | PRO  | N-CD  | -10.13 | 1.33        | 1.47     |
| 10  | C32   | 680  | ALA  | C-N   | 10.13  | 1.47        | 1.33     |
| 19  | 48    | 91   | PRO  | N-CD  | -10.13 | 1.33        | 1.47     |
| 7   | Q8    | 222  | PHE  | C-N   | -10.13 | 1.19        | 1.33     |
| 10  | C16   | 907  | PRO  | N-CD  | -10.13 | 1.33        | 1.47     |
| 10  | C     | 1802 | PRO  | N-CD  | -10.13 | 1.33        | 1.47     |
| 7   | Q16   | 222  | PHE  | C-N   | -10.13 | 1.19        | 1.33     |
| 23  | J16   | 681  | GLU  | C-N   | 10.12  | 1.47        | 1.33     |
| 10  | C     | 680  | ALA  | C-N   | 10.12  | 1.46        | 1.33     |
| 10  | C32   | 1802 | PRO  | N-CD  | -10.12 | 1.33        | 1.47     |
| 5   | P     | 65   | GLY  | C-N   | 10.11  | 1.45        | 1.33     |
| 10  | C24   | 536  | PRO  | N-CD  | -10.11 | 1.33        | 1.47     |
| 10  | C     | 1292 | SER  | C-N   | -10.11 | 1.20        | 1.33     |
| 23  | J24   | 681  | GLU  | C-N   | 10.11  | 1.47        | 1.33     |
| 10  | C24   | 680  | ALA  | C-N   | 10.10  | 1.46        | 1.33     |
| 18  | B     | 157  | PRO  | N-CD  | -10.10 | 1.33        | 1.47     |
| 10  | C24   | 23   | PRO  | N-CD  | -10.10 | 1.33        | 1.47     |
| 10  | C8    | 536  | PRO  | N-CD  | -10.10 | 1.33        | 1.47     |
| 10  | C16   | 489  | THR  | C-N   | -10.08 | 1.21        | 1.33     |
| 10  | C8    | 489  | THR  | C-N   | -10.08 | 1.21        | 1.33     |
| 19  | 48    | 190  | ARG  | C-N   | -10.08 | 1.20        | 1.33     |
| 1   | R16   | 1224 | VAL  | C-N   | -10.07 | 1.20        | 1.33     |
| 10  | C     | 23   | PRO  | N-CD  | -10.06 | 1.33        | 1.47     |
| 18  | B8    | 157  | PRO  | N-CD  | -10.06 | 1.33        | 1.47     |
| 23  | J32   | 681  | GLU  | C-N   | 10.06  | 1.47        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 5   | P8    | 65   | GLY  | C-N   | 10.06  | 1.45        | 1.33     |
| 9   | K8    | 721  | PRO  | N-CD  | -10.06 | 1.33        | 1.47     |
| 10  | C     | 489  | THR  | C-N   | -10.06 | 1.21        | 1.33     |
| 18  | B8    | 1128 | PRO  | N-CD  | -10.05 | 1.33        | 1.47     |
| 19  | 4     | 190  | ARG  | C-N   | -10.05 | 1.20        | 1.33     |
| 10  | C32   | 489  | THR  | C-N   | -10.05 | 1.21        | 1.33     |
| 7   | Q     | 222  | PHE  | C-N   | -10.05 | 1.19        | 1.33     |
| 10  | C16   | 1670 | PRO  | N-CD  | -10.04 | 1.33        | 1.47     |
| 9   | K     | 721  | PRO  | N-CD  | -10.04 | 1.33        | 1.47     |
| 18  | B     | 870  | PRO  | N-CD  | -10.04 | 1.33        | 1.47     |
| 18  | B     | 1128 | PRO  | N-CD  | -10.04 | 1.33        | 1.47     |
| 18  | B8    | 870  | PRO  | N-CD  | -10.03 | 1.33        | 1.47     |
| 9   | K8    | 1090 | ASP  | C-N   | 10.03  | 1.45        | 1.33     |
| 10  | C24   | 1802 | PRO  | N-CD  | -10.03 | 1.33        | 1.47     |
| 10  | C16   | 536  | PRO  | N-CD  | -10.02 | 1.33        | 1.47     |
| 10  | C16   | 1802 | PRO  | N-CD  | -10.02 | 1.33        | 1.47     |
| 5   | P16   | 65   | GLY  | C-N   | 10.01  | 1.45        | 1.33     |
| 15  | J     | 595  | THR  | C-N   | -10.01 | 1.20        | 1.33     |
| 10  | C8    | 330  | GLY  | C-N   | 10.01  | 1.46        | 1.33     |
| 23  | J8    | 681  | GLU  | C-N   | 10.00  | 1.47        | 1.33     |
| 10  | C8    | 1670 | PRO  | N-CD  | -9.99  | 1.33        | 1.47     |
| 10  | C24   | 1774 | SER  | C-N   | -9.99  | 1.23        | 1.34     |
| 10  | C32   | 536  | PRO  | N-CD  | -9.99  | 1.33        | 1.47     |
| 9   | K     | 1090 | ASP  | C-N   | 9.99   | 1.45        | 1.33     |
| 10  | C     | 536  | PRO  | N-CD  | -9.98  | 1.33        | 1.47     |
| 7   | Q     | 66   | PRO  | N-CD  | -9.97  | 1.33        | 1.47     |
| 10  | C24   | 489  | THR  | C-N   | -9.96  | 1.21        | 1.33     |
| 10  | C     | 1670 | PRO  | N-CD  | -9.96  | 1.33        | 1.47     |
| 10  | C16   | 1774 | SER  | C-N   | -9.96  | 1.23        | 1.34     |
| 10  | C32   | 1670 | PRO  | N-CD  | -9.96  | 1.33        | 1.47     |
| 18  | B     | 1838 | ALA  | C-N   | -9.96  | 1.20        | 1.33     |
| 7   | Q8    | 66   | PRO  | N-CD  | -9.94  | 1.33        | 1.47     |
| 13  | V     | 752  | GLY  | C-N   | 9.94   | 1.44        | 1.33     |
| 13  | V     | 881  | GLY  | C-N   | 9.94   | 1.44        | 1.33     |
| 18  | B     | 1230 | GLY  | C-N   | 9.94   | 1.47        | 1.33     |
| 20  | E     | 4    | PRO  | N-CD  | -9.92  | 1.33        | 1.47     |
| 7   | Q16   | 66   | PRO  | N-CD  | -9.92  | 1.33        | 1.47     |
| 11  | A40   | 57   | PRO  | C-N   | -9.91  | 1.19        | 1.33     |
| 10  | C8    | 1774 | SER  | C-N   | -9.91  | 1.23        | 1.34     |
| 19  | 4     | 207  | LEU  | C-N   | -9.91  | 1.19        | 1.33     |
| 11  | A16   | 57   | PRO  | C-N   | -9.91  | 1.19        | 1.33     |
| 18  | B8    | 1838 | ALA  | C-N   | -9.91  | 1.20        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 669  | GLY  | C-N   | 9.90  | 1.41        | 1.33     |
| 11  | A24   | 57   | PRO  | C-N   | -9.90 | 1.19        | 1.33     |
| 10  | C32   | 1774 | SER  | C-N   | -9.90 | 1.23        | 1.34     |
| 11  | A40   | 736  | PRO  | N-CD  | -9.90 | 1.33        | 1.47     |
| 18  | B     | 1449 | ALA  | C-N   | -9.89 | 1.22        | 1.33     |
| 18  | B8    | 1230 | GLY  | C-N   | 9.89  | 1.47        | 1.33     |
| 19  | 48    | 207  | LEU  | C-N   | -9.89 | 1.19        | 1.33     |
| 18  | B8    | 906  | SER  | C-N   | 9.88  | 1.46        | 1.33     |
| 18  | B     | 1127 | PRO  | N-CD  | -9.88 | 1.33        | 1.47     |
| 18  | B8    | 1127 | PRO  | N-CD  | -9.88 | 1.33        | 1.47     |
| 10  | C24   | 1670 | PRO  | N-CD  | -9.87 | 1.33        | 1.47     |
| 13  | V     | 747  | SER  | C-N   | -9.87 | 1.21        | 1.33     |
| 9   | K     | 828  | PRO  | N-CD  | -9.87 | 1.33        | 1.47     |
| 20  | E8    | 4    | PRO  | N-CD  | -9.86 | 1.33        | 1.47     |
| 9   | K     | 822  | PRO  | N-CD  | -9.86 | 1.33        | 1.47     |
| 10  | C24   | 669  | GLY  | C-N   | 9.86  | 1.41        | 1.33     |
| 18  | B     | 1786 | PRO  | N-CD  | -9.85 | 1.33        | 1.47     |
| 9   | K8    | 822  | PRO  | N-CD  | -9.85 | 1.33        | 1.47     |
| 18  | B     | 906  | SER  | C-N   | 9.84  | 1.46        | 1.33     |
| 13  | V     | 830  | GLN  | C-N   | -9.83 | 1.20        | 1.33     |
| 22  | I     | 370  | PRO  | N-CD  | -9.83 | 1.33        | 1.47     |
| 7   | Q16   | 26   | PRO  | N-CD  | -9.82 | 1.34        | 1.47     |
| 11  | A32   | 57   | PRO  | C-N   | -9.81 | 1.19        | 1.33     |
| 18  | B8    | 1734 | LYS  | C-N   | -9.81 | 1.20        | 1.33     |
| 19  | 48    | 183  | ARG  | C-N   | 9.80  | 1.46        | 1.33     |
| 10  | C16   | 182  | ASP  | C-N   | -9.80 | 1.22        | 1.33     |
| 22  | I16   | 370  | PRO  | N-CD  | -9.79 | 1.34        | 1.47     |
| 5   | P8    | 480  | PRO  | N-CD  | 9.79  | 1.61        | 1.47     |
| 10  | C     | 182  | ASP  | C-N   | -9.79 | 1.22        | 1.33     |
| 11  | A32   | 736  | PRO  | N-CD  | -9.79 | 1.34        | 1.47     |
| 9   | K8    | 828  | PRO  | N-CD  | -9.79 | 1.34        | 1.47     |
| 10  | C8    | 182  | ASP  | C-N   | -9.79 | 1.22        | 1.33     |
| 19  | 4     | 183  | ARG  | C-N   | 9.79  | 1.46        | 1.33     |
| 3   | N8    | 60   | TRP  | C-N   | 9.78  | 1.47        | 1.33     |
| 7   | Q     | 26   | PRO  | N-CD  | -9.78 | 1.34        | 1.47     |
| 10  | C     | 1774 | SER  | C-N   | -9.78 | 1.23        | 1.34     |
| 10  | C32   | 182  | ASP  | C-N   | -9.78 | 1.22        | 1.33     |
| 23  | J16   | 724  | GLY  | C-N   | 9.77  | 1.47        | 1.33     |
| 9   | K     | 1129 | PRO  | N-CD  | -9.77 | 1.34        | 1.47     |
| 5   | P     | 480  | PRO  | N-CD  | 9.77  | 1.61        | 1.47     |
| 10  | C24   | 182  | ASP  | C-N   | -9.77 | 1.22        | 1.33     |
| 22  | I24   | 370  | PRO  | N-CD  | -9.77 | 1.34        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C8    | 1079 | THR  | C-N   | 9.76  | 1.47        | 1.33     |
| 18  | B8    | 1786 | PRO  | N-CD  | -9.76 | 1.34        | 1.47     |
| 10  | C32   | 669  | GLY  | C-N   | 9.76  | 1.41        | 1.33     |
| 18  | B8    | 1449 | ALA  | C-N   | -9.75 | 1.22        | 1.33     |
| 10  | C24   | 331  | ILE  | C-N   | 9.75  | 1.47        | 1.33     |
| 23  | J32   | 724  | GLY  | C-N   | 9.75  | 1.47        | 1.33     |
| 2   | M8    | 814  | PRO  | N-CD  | -9.74 | 1.34        | 1.47     |
| 9   | K8    | 1232 | LEU  | C-N   | 9.74  | 1.47        | 1.33     |
| 10  | C     | 669  | GLY  | C-N   | 9.74  | 1.41        | 1.33     |
| 5   | P16   | 480  | PRO  | N-CD  | 9.74  | 1.61        | 1.47     |
| 18  | B     | 1734 | LYS  | C-N   | -9.74 | 1.21        | 1.33     |
| 11  | A24   | 736  | PRO  | N-CD  | -9.73 | 1.34        | 1.47     |
| 7   | Q8    | 26   | PRO  | N-CD  | -9.73 | 1.34        | 1.47     |
| 9   | K8    | 1129 | PRO  | N-CD  | -9.73 | 1.34        | 1.47     |
| 2   | M     | 814  | PRO  | N-CD  | -9.73 | 1.34        | 1.47     |
| 3   | N     | 60   | TRP  | C-N   | 9.73  | 1.47        | 1.33     |
| 10  | C     | 1079 | THR  | C-N   | 9.73  | 1.47        | 1.33     |
| 11  | A16   | 736  | PRO  | N-CD  | -9.72 | 1.34        | 1.47     |
| 2   | M16   | 814  | PRO  | N-CD  | -9.72 | 1.34        | 1.47     |
| 10  | C16   | 1079 | THR  | C-N   | 9.72  | 1.47        | 1.33     |
| 10  | C     | 331  | ILE  | C-N   | 9.72  | 1.47        | 1.33     |
| 10  | C8    | 307  | PRO  | N-CD  | -9.72 | 1.34        | 1.47     |
| 10  | C24   | 307  | PRO  | N-CD  | -9.72 | 1.34        | 1.47     |
| 11  | A40   | 53   | ARG  | C-N   | 9.71  | 1.46        | 1.33     |
| 3   | N16   | 60   | TRP  | C-N   | 9.71  | 1.46        | 1.33     |
| 10  | C8    | 669  | GLY  | C-N   | 9.71  | 1.41        | 1.33     |
| 18  | B8    | 1745 | HIS  | C-N   | -9.71 | 1.20        | 1.33     |
| 22  | I8    | 370  | PRO  | N-CD  | -9.70 | 1.34        | 1.47     |
| 10  | C24   | 1079 | THR  | C-N   | 9.70  | 1.47        | 1.33     |
| 10  | C16   | 331  | ILE  | C-N   | 9.69  | 1.47        | 1.33     |
| 18  | B     | 1745 | HIS  | C-N   | -9.69 | 1.20        | 1.33     |
| 1   | R16   | 1185 | THR  | C-N   | -9.69 | 1.20        | 1.33     |
| 10  | C16   | 438  | PRO  | N-CD  | -9.69 | 1.34        | 1.47     |
| 23  | J24   | 724  | GLY  | C-N   | 9.69  | 1.47        | 1.33     |
| 23  | J8    | 724  | GLY  | C-N   | 9.68  | 1.47        | 1.33     |
| 12  | A     | 736  | PRO  | N-CD  | -9.67 | 1.34        | 1.47     |
| 1   | R     | 1185 | THR  | C-N   | -9.67 | 1.20        | 1.33     |
| 12  | A48   | 736  | PRO  | N-CD  | -9.67 | 1.34        | 1.47     |
| 9   | K     | 1232 | LEU  | C-N   | 9.66  | 1.47        | 1.33     |
| 10  | C16   | 307  | PRO  | N-CD  | -9.66 | 1.34        | 1.47     |
| 10  | C32   | 307  | PRO  | N-CD  | -9.65 | 1.34        | 1.47     |
| 10  | C     | 307  | PRO  | N-CD  | -9.64 | 1.34        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A16   | 53   | ARG  | C-N   | 9.63  | 1.46        | 1.33     |
| 7   | Q     | 12   | ARG  | C-N   | -9.62 | 1.23        | 1.33     |
| 10  | C32   | 1079 | THR  | C-N   | 9.62  | 1.47        | 1.33     |
| 18  | B     | 1811 | PRO  | N-CD  | -9.62 | 1.34        | 1.47     |
| 10  | C8    | 331  | ILE  | C-N   | 9.62  | 1.47        | 1.33     |
| 11  | A24   | 53   | ARG  | C-N   | 9.61  | 1.46        | 1.33     |
| 10  | C24   | 438  | PRO  | N-CD  | -9.61 | 1.34        | 1.47     |
| 10  | C32   | 331  | ILE  | C-N   | 9.61  | 1.47        | 1.33     |
| 10  | C32   | 438  | PRO  | N-CD  | -9.60 | 1.34        | 1.47     |
| 9   | K     | 1064 | PRO  | N-CD  | -9.60 | 1.34        | 1.47     |
| 10  | C     | 438  | PRO  | N-CD  | -9.60 | 1.34        | 1.47     |
| 10  | C24   | 1730 | ILE  | C-N   | -9.57 | 1.21        | 1.33     |
| 10  | C24   | 4    | PRO  | C-N   | -9.57 | 1.21        | 1.33     |
| 18  | B     | 1591 | MET  | C-N   | -9.57 | 1.19        | 1.33     |
| 20  | E     | 446  | PRO  | N-CD  | -9.57 | 1.34        | 1.47     |
| 9   | K8    | 1064 | PRO  | N-CD  | -9.57 | 1.34        | 1.47     |
| 11  | A32   | 53   | ARG  | C-N   | 9.57  | 1.46        | 1.33     |
| 10  | C8    | 48   | PRO  | C-N   | -9.56 | 1.22        | 1.33     |
| 18  | B8    | 1591 | MET  | C-N   | -9.56 | 1.19        | 1.33     |
| 1   | R8    | 1185 | THR  | C-N   | -9.56 | 1.20        | 1.33     |
| 18  | B8    | 1811 | PRO  | N-CD  | -9.56 | 1.34        | 1.47     |
| 18  | B8    | 1685 | THR  | C-N   | -9.56 | 1.20        | 1.33     |
| 10  | C32   | 104  | GLU  | C-N   | 9.55  | 1.48        | 1.33     |
| 10  | C8    | 438  | PRO  | N-CD  | -9.55 | 1.34        | 1.47     |
| 20  | E8    | 446  | PRO  | N-CD  | -9.55 | 1.34        | 1.47     |
| 9   | K8    | 1278 | GLU  | C-N   | 9.54  | 1.47        | 1.34     |
| 13  | V     | 795  | GLN  | C-N   | -9.54 | 1.21        | 1.33     |
| 18  | B     | 1685 | THR  | C-N   | -9.54 | 1.20        | 1.33     |
| 7   | Q16   | 12   | ARG  | C-N   | -9.53 | 1.24        | 1.33     |
| 15  | J     | 543  | VAL  | C-N   | -9.52 | 1.21        | 1.33     |
| 10  | C8    | 4    | PRO  | C-N   | -9.52 | 1.21        | 1.33     |
| 13  | V     | 819  | ALA  | C-N   | 9.51  | 1.47        | 1.33     |
| 10  | C32   | 48   | PRO  | C-N   | -9.51 | 1.22        | 1.33     |
| 10  | C16   | 4    | PRO  | C-N   | -9.50 | 1.21        | 1.33     |
| 10  | C16   | 1730 | ILE  | C-N   | -9.50 | 1.21        | 1.33     |
| 18  | B8    | 1600 | LEU  | C-N   | 9.50  | 1.45        | 1.33     |
| 18  | B     | 1753 | PRO  | C-N   | -9.50 | 1.22        | 1.33     |
| 10  | C24   | 671  | LYS  | C-N   | 9.49  | 1.49        | 1.33     |
| 19  | 48    | 332  | PRO  | N-CD  | 9.49  | 1.61        | 1.47     |
| 9   | K8    | 1158 | SER  | C-N   | -9.49 | 1.20        | 1.34     |
| 12  | A48   | 241  | VAL  | C-N   | 9.49  | 1.47        | 1.33     |
| 9   | K     | 1278 | GLU  | C-N   | 9.48  | 1.47        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 15  | J     | 684  | ASP  | C-N   | 9.48  | 1.47        | 1.33     |
| 18  | B     | 1634 | LEU  | C-N   | 9.48  | 1.46        | 1.33     |
| 18  | B8    | 1753 | PRO  | C-N   | -9.48 | 1.22        | 1.33     |
| 18  | B     | 1600 | LEU  | C-N   | 9.48  | 1.45        | 1.33     |
| 14  | W     | 641  | GLU  | C-N   | -9.48 | 1.21        | 1.33     |
| 10  | C24   | 48   | PRO  | C-N   | -9.47 | 1.22        | 1.33     |
| 7   | Q8    | 12   | ARG  | C-N   | -9.47 | 1.24        | 1.33     |
| 10  | C     | 1730 | ILE  | C-N   | -9.47 | 1.21        | 1.33     |
| 11  | A32   | 241  | VAL  | C-N   | 9.47  | 1.47        | 1.33     |
| 10  | C32   | 4    | PRO  | C-N   | -9.47 | 1.21        | 1.33     |
| 12  | A48   | 824  | PRO  | N-CD  | -9.47 | 1.34        | 1.47     |
| 18  | B8    | 1634 | LEU  | C-N   | 9.46  | 1.45        | 1.33     |
| 11  | A24   | 824  | PRO  | N-CD  | -9.45 | 1.34        | 1.47     |
| 10  | C     | 628  | GLY  | C-N   | 9.45  | 1.47        | 1.33     |
| 19  | 4     | 332  | PRO  | N-CD  | 9.45  | 1.61        | 1.47     |
| 10  | C8    | 104  | GLU  | C-N   | 9.45  | 1.48        | 1.33     |
| 7   | Q16   | 164  | ASN  | C-N   | -9.45 | 1.19        | 1.33     |
| 10  | C     | 48   | PRO  | C-N   | -9.45 | 1.22        | 1.33     |
| 10  | C16   | 671  | LYS  | C-N   | 9.44  | 1.49        | 1.33     |
| 10  | C32   | 671  | LYS  | C-N   | 9.44  | 1.49        | 1.33     |
| 9   | K     | 718  | PHE  | C-N   | 9.44  | 1.47        | 1.33     |
| 11  | A16   | 824  | PRO  | N-CD  | -9.44 | 1.34        | 1.47     |
| 12  | A     | 241  | VAL  | C-N   | 9.44  | 1.46        | 1.33     |
| 9   | K8    | 1099 | ARG  | C-N   | -9.43 | 1.22        | 1.33     |
| 12  | A     | 824  | PRO  | N-CD  | -9.43 | 1.34        | 1.47     |
| 11  | A16   | 241  | VAL  | C-N   | 9.43  | 1.46        | 1.33     |
| 10  | C24   | 104  | GLU  | C-N   | 9.43  | 1.48        | 1.33     |
| 11  | A32   | 824  | PRO  | N-CD  | -9.41 | 1.34        | 1.47     |
| 9   | K     | 1158 | SER  | C-N   | -9.41 | 1.21        | 1.34     |
| 10  | C     | 4    | PRO  | C-N   | -9.41 | 1.21        | 1.33     |
| 10  | C     | 104  | GLU  | C-N   | 9.41  | 1.48        | 1.33     |
| 18  | B     | 1505 | MET  | C-N   | 9.41  | 1.45        | 1.33     |
| 10  | C     | 671  | LYS  | C-N   | 9.40  | 1.49        | 1.33     |
| 7   | Q16   | 91   | GLY  | C-N   | 9.40  | 1.47        | 1.33     |
| 11  | A40   | 824  | PRO  | N-CD  | -9.40 | 1.34        | 1.47     |
| 10  | C24   | 1156 | LYS  | C-N   | -9.39 | 1.21        | 1.34     |
| 9   | K8    | 718  | PHE  | C-N   | 9.38  | 1.47        | 1.33     |
| 11  | A40   | 241  | VAL  | C-N   | 9.38  | 1.46        | 1.33     |
| 7   | Q8    | 164  | ASN  | C-N   | -9.38 | 1.19        | 1.33     |
| 10  | C8    | 671  | LYS  | C-N   | 9.38  | 1.49        | 1.33     |
| 20  | E8    | 363  | SER  | C-N   | -9.37 | 1.21        | 1.33     |
| 10  | C32   | 628  | GLY  | C-N   | 9.37  | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 1730 | ILE  | C-N   | -9.37 | 1.22        | 1.33     |
| 10  | C16   | 104  | GLU  | C-N   | 9.37  | 1.48        | 1.33     |
| 20  | E     | 363  | SER  | C-N   | -9.37 | 1.21        | 1.33     |
| 10  | C8    | 1730 | ILE  | C-N   | -9.36 | 1.22        | 1.33     |
| 11  | A24   | 241  | VAL  | C-N   | 9.36  | 1.46        | 1.33     |
| 7   | Q8    | 91   | GLY  | C-N   | 9.35  | 1.47        | 1.33     |
| 10  | C16   | 48   | PRO  | C-N   | -9.35 | 1.22        | 1.33     |
| 10  | C32   | 1156 | LYS  | C-N   | -9.34 | 1.21        | 1.34     |
| 10  | C16   | 628  | GLY  | C-N   | 9.34  | 1.46        | 1.33     |
| 10  | C     | 1156 | LYS  | C-N   | -9.33 | 1.21        | 1.34     |
| 7   | Q     | 91   | GLY  | C-N   | 9.32  | 1.47        | 1.33     |
| 9   | K     | 1099 | ARG  | C-N   | -9.32 | 1.22        | 1.33     |
| 10  | C8    | 279  | LEU  | C-N   | 9.32  | 1.47        | 1.33     |
| 20  | E     | 2    | PRO  | N-CD  | -9.32 | 1.34        | 1.47     |
| 20  | E8    | 2    | PRO  | N-CD  | -9.32 | 1.34        | 1.47     |
| 18  | B8    | 521  | PRO  | N-CD  | -9.31 | 1.34        | 1.47     |
| 18  | B8    | 1505 | MET  | C-N   | 9.31  | 1.45        | 1.33     |
| 10  | C32   | 279  | LEU  | C-N   | 9.31  | 1.47        | 1.33     |
| 10  | C24   | 628  | GLY  | C-N   | 9.30  | 1.46        | 1.33     |
| 10  | C16   | 279  | LEU  | C-N   | 9.30  | 1.47        | 1.33     |
| 10  | C24   | 279  | LEU  | C-N   | 9.28  | 1.47        | 1.33     |
| 7   | Q     | 164  | ASN  | C-N   | -9.28 | 1.19        | 1.33     |
| 10  | C     | 279  | LEU  | C-N   | 9.28  | 1.47        | 1.33     |
| 18  | B8    | 442  | SER  | C-N   | -9.28 | 1.20        | 1.33     |
| 10  | C16   | 1156 | LYS  | C-N   | -9.27 | 1.21        | 1.34     |
| 10  | C8    | 1156 | LYS  | C-N   | -9.26 | 1.21        | 1.34     |
| 19  | 48    | 288  | SER  | C-N   | -9.26 | 1.23        | 1.33     |
| 5   | P16   | 260  | GLN  | C-N   | -9.25 | 1.21        | 1.33     |
| 10  | C     | 1080 | SER  | C-N   | -9.24 | 1.20        | 1.33     |
| 18  | B     | 1448 | ASN  | C-N   | 9.24  | 1.46        | 1.33     |
| 10  | C24   | 1080 | SER  | C-N   | -9.23 | 1.20        | 1.33     |
| 18  | B     | 521  | PRO  | N-CD  | -9.23 | 1.34        | 1.47     |
| 18  | B8    | 1448 | ASN  | C-N   | 9.22  | 1.46        | 1.33     |
| 10  | C24   | 1658 | ASP  | C-N   | 9.22  | 1.45        | 1.33     |
| 5   | P     | 260  | GLN  | C-N   | -9.22 | 1.21        | 1.33     |
| 18  | B     | 537  | LEU  | C-N   | 9.22  | 1.45        | 1.33     |
| 5   | P8    | 260  | GLN  | C-N   | -9.21 | 1.21        | 1.33     |
| 9   | K8    | 1080 | LEU  | C-N   | -9.21 | 1.21        | 1.33     |
| 10  | C8    | 1080 | SER  | C-N   | -9.21 | 1.20        | 1.33     |
| 6   | O16   | 107  | SER  | C-N   | -9.21 | 1.22        | 1.33     |
| 18  | B     | 937  | ASP  | C-N   | 9.20  | 1.45        | 1.33     |
| 10  | C16   | 724  | SER  | C-N   | -9.20 | 1.21        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 442  | SER  | C-N   | -9.20 | 1.20        | 1.33     |
| 19  | 4     | 288  | SER  | C-N   | -9.19 | 1.24        | 1.33     |
| 18  | B8    | 537  | LEU  | C-N   | 9.18  | 1.45        | 1.33     |
| 10  | C     | 1620 | ILE  | C-N   | 9.18  | 1.45        | 1.33     |
| 19  | 4     | 392  | ILE  | C-N   | -9.17 | 1.23        | 1.33     |
| 18  | B8    | 937  | ASP  | C-N   | 9.16  | 1.45        | 1.33     |
| 9   | K     | 1163 | HIS  | C-N   | -9.16 | 1.21        | 1.33     |
| 10  | C32   | 724  | SER  | C-N   | -9.15 | 1.22        | 1.33     |
| 10  | C32   | 1080 | SER  | C-N   | -9.15 | 1.20        | 1.33     |
| 19  | 48    | 392  | ILE  | C-N   | -9.15 | 1.23        | 1.33     |
| 2   | M     | 753  | ALA  | C-N   | 9.14  | 1.46        | 1.33     |
| 10  | C16   | 1658 | ASP  | C-N   | 9.14  | 1.45        | 1.33     |
| 10  | C8    | 1620 | ILE  | C-N   | 9.14  | 1.45        | 1.33     |
| 10  | C     | 1658 | ASP  | C-N   | 9.13  | 1.45        | 1.33     |
| 10  | C16   | 1080 | SER  | C-N   | -9.12 | 1.21        | 1.33     |
| 2   | M8    | 753  | ALA  | C-N   | 9.12  | 1.46        | 1.33     |
| 18  | B     | 1527 | THR  | C-N   | 9.12  | 1.45        | 1.33     |
| 20  | E     | 355  | PRO  | N-CD  | -9.11 | 1.34        | 1.47     |
| 20  | E     | 449  | ARG  | C-N   | 9.11  | 1.46        | 1.34     |
| 10  | C8    | 1599 | ASP  | C-N   | 9.11  | 1.44        | 1.33     |
| 10  | C16   | 105  | TRP  | C-N   | -9.10 | 1.20        | 1.33     |
| 10  | C24   | 856  | PRO  | N-CD  | -9.10 | 1.35        | 1.47     |
| 10  | C     | 724  | SER  | C-N   | -9.10 | 1.22        | 1.33     |
| 1   | R16   | 1179 | ASP  | C-N   | -9.09 | 1.22        | 1.33     |
| 10  | C8    | 856  | PRO  | N-CD  | -9.09 | 1.35        | 1.47     |
| 20  | E8    | 355  | PRO  | N-CD  | -9.09 | 1.35        | 1.47     |
| 11  | A24   | 619  | MET  | C-N   | -9.09 | 1.22        | 1.33     |
| 1   | R16   | 1247 | PRO  | N-CD  | -9.09 | 1.35        | 1.47     |
| 6   | O     | 107  | SER  | C-N   | -9.09 | 1.22        | 1.33     |
| 12  | A48   | 619  | MET  | C-N   | -9.09 | 1.22        | 1.33     |
| 3   | N16   | 164  | PRO  | N-CD  | -9.08 | 1.35        | 1.47     |
| 9   | K8    | 1069 | PRO  | N-CD  | -9.08 | 1.35        | 1.47     |
| 9   | K8    | 1163 | HIS  | C-N   | -9.08 | 1.21        | 1.33     |
| 10  | C24   | 1620 | ILE  | C-N   | 9.08  | 1.45        | 1.33     |
| 5   | P     | 614  | VAL  | C-N   | -9.07 | 1.21        | 1.34     |
| 11  | A32   | 619  | MET  | C-N   | -9.07 | 1.22        | 1.33     |
| 5   | P16   | 614  | VAL  | C-N   | -9.07 | 1.21        | 1.34     |
| 10  | C16   | 1620 | ILE  | C-N   | 9.07  | 1.45        | 1.33     |
| 9   | K8    | 1062 | PRO  | N-CD  | -9.07 | 1.35        | 1.47     |
| 10  | C8    | 2    | VAL  | C-N   | -9.07 | 1.19        | 1.33     |
| 10  | C8    | 833  | PRO  | N-CD  | -9.07 | 1.35        | 1.47     |
| 10  | C32   | 105  | TRP  | C-N   | -9.06 | 1.20        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 1216 | PRO  | N-CD  | -9.06 | 1.35        | 1.47     |
| 10  | C     | 833  | PRO  | N-CD  | -9.06 | 1.35        | 1.47     |
| 6   | O8    | 107  | SER  | C-N   | -9.06 | 1.22        | 1.33     |
| 19  | 4     | 154  | PRO  | N-CD  | -9.06 | 1.35        | 1.47     |
| 1   | R     | 1179 | ASP  | C-N   | -9.05 | 1.22        | 1.33     |
| 20  | E8    | 449  | ARG  | C-N   | 9.05  | 1.46        | 1.34     |
| 9   | K     | 1062 | PRO  | N-CD  | -9.05 | 1.35        | 1.47     |
| 10  | C16   | 856  | PRO  | N-CD  | -9.05 | 1.35        | 1.47     |
| 11  | A40   | 90   | PHE  | C-N   | 9.05  | 1.46        | 1.33     |
| 11  | A24   | 90   | PHE  | C-N   | 9.04  | 1.46        | 1.33     |
| 10  | C24   | 833  | PRO  | N-CD  | -9.04 | 1.35        | 1.47     |
| 11  | A40   | 619  | MET  | C-N   | -9.04 | 1.22        | 1.33     |
| 1   | R8    | 1179 | ASP  | C-N   | -9.04 | 1.22        | 1.33     |
| 2   | M16   | 753  | ALA  | C-N   | 9.04  | 1.46        | 1.33     |
| 9   | K8    | 1187 | SER  | C-N   | 9.04  | 1.46        | 1.33     |
| 10  | C24   | 1599 | ASP  | C-N   | 9.04  | 1.44        | 1.33     |
| 10  | C     | 1447 | LEU  | C-N   | 9.04  | 1.46        | 1.33     |
| 11  | A16   | 619  | MET  | C-N   | -9.03 | 1.22        | 1.33     |
| 10  | C24   | 724  | SER  | C-N   | -9.03 | 1.22        | 1.33     |
| 7   | Q     | 260  | PRO  | N-CD  | -9.02 | 1.35        | 1.47     |
| 9   | K8    | 1280 | PHE  | C-N   | 9.02  | 1.45        | 1.33     |
| 3   | N8    | 164  | PRO  | N-CD  | -9.02 | 1.35        | 1.47     |
| 12  | A     | 619  | MET  | C-N   | -9.02 | 1.22        | 1.33     |
| 9   | K     | 1187 | SER  | C-N   | 9.02  | 1.46        | 1.33     |
| 10  | C16   | 1599 | ASP  | C-N   | 9.02  | 1.44        | 1.33     |
| 10  | C8    | 358  | LYS  | C-N   | -9.02 | 1.21        | 1.33     |
| 11  | A32   | 90   | PHE  | C-N   | 9.02  | 1.46        | 1.33     |
| 7   | Q16   | 260  | PRO  | N-CD  | -9.02 | 1.35        | 1.47     |
| 1   | R8    | 1247 | PRO  | N-CD  | -9.02 | 1.35        | 1.47     |
| 18  | B8    | 28   | LEU  | C-N   | 9.02  | 1.47        | 1.33     |
| 9   | K     | 709  | MET  | C-N   | -9.01 | 1.22        | 1.33     |
| 1   | R     | 1247 | PRO  | N-CD  | -9.01 | 1.35        | 1.47     |
| 10  | C8    | 105  | TRP  | C-N   | -9.01 | 1.20        | 1.33     |
| 18  | B     | 866  | SER  | C-N   | 9.01  | 1.46        | 1.33     |
| 19  | 48    | 154  | PRO  | N-CD  | -9.01 | 1.35        | 1.47     |
| 10  | C32   | 2    | VAL  | C-N   | -9.01 | 1.19        | 1.33     |
| 9   | K     | 1080 | LEU  | C-N   | -9.01 | 1.22        | 1.33     |
| 10  | C     | 1599 | ASP  | C-N   | 9.01  | 1.44        | 1.33     |
| 9   | K     | 1069 | PRO  | N-CD  | -9.01 | 1.35        | 1.47     |
| 10  | C32   | 1286 | MET  | C-N   | 9.00  | 1.45        | 1.33     |
| 10  | C24   | 105  | TRP  | C-N   | -9.00 | 1.20        | 1.33     |
| 7   | Q8    | 260  | PRO  | N-CD  | -9.00 | 1.35        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 2    | VAL  | C-N   | -9.00 | 1.19        | 1.33     |
| 10  | C24   | 1286 | MET  | C-N   | 8.99  | 1.45        | 1.33     |
| 10  | C16   | 148  | GLU  | C-N   | -8.99 | 1.20        | 1.33     |
| 11  | A16   | 90   | PHE  | C-N   | 8.99  | 1.46        | 1.33     |
| 10  | C16   | 1671 | THR  | C-N   | -8.99 | 1.22        | 1.34     |
| 10  | C32   | 1447 | LEU  | C-N   | 8.99  | 1.46        | 1.33     |
| 10  | C32   | 1658 | ASP  | C-N   | 8.99  | 1.45        | 1.33     |
| 10  | C     | 2    | VAL  | C-N   | -8.99 | 1.19        | 1.33     |
| 10  | C     | 105  | TRP  | C-N   | -8.98 | 1.20        | 1.33     |
| 10  | C8    | 1447 | LEU  | C-N   | 8.98  | 1.46        | 1.33     |
| 10  | C32   | 833  | PRO  | N-CD  | -8.98 | 1.35        | 1.47     |
| 10  | C32   | 856  | PRO  | N-CD  | -8.98 | 1.35        | 1.47     |
| 10  | C32   | 1599 | ASP  | C-N   | 8.98  | 1.44        | 1.33     |
| 10  | C24   | 1447 | LEU  | C-N   | 8.98  | 1.46        | 1.33     |
| 14  | W     | 686  | GLU  | C-N   | -8.98 | 1.21        | 1.33     |
| 10  | C8    | 1286 | MET  | C-N   | 8.97  | 1.45        | 1.33     |
| 10  | C     | 856  | PRO  | N-CD  | -8.97 | 1.35        | 1.47     |
| 10  | C     | 1286 | MET  | C-N   | 8.97  | 1.45        | 1.33     |
| 18  | B8    | 1527 | THR  | C-N   | 8.97  | 1.45        | 1.33     |
| 10  | C32   | 1620 | ILE  | C-N   | 8.97  | 1.45        | 1.33     |
| 18  | B8    | 294  | PHE  | C-N   | 8.97  | 1.46        | 1.34     |
| 18  | B8    | 866  | SER  | C-N   | 8.97  | 1.46        | 1.33     |
| 3   | N     | 164  | PRO  | N-CD  | -8.97 | 1.35        | 1.47     |
| 9   | K     | 1280 | PHE  | C-N   | 8.96  | 1.45        | 1.33     |
| 10  | C16   | 1286 | MET  | C-N   | 8.96  | 1.45        | 1.33     |
| 10  | C8    | 1671 | THR  | C-N   | -8.96 | 1.22        | 1.34     |
| 10  | C32   | 358  | LYS  | C-N   | -8.96 | 1.21        | 1.33     |
| 10  | C24   | 716  | THR  | C-N   | 8.96  | 1.46        | 1.34     |
| 10  | C16   | 2    | VAL  | C-N   | -8.95 | 1.19        | 1.33     |
| 10  | C24   | 1671 | THR  | C-N   | -8.94 | 1.22        | 1.34     |
| 10  | C8    | 148  | GLU  | C-N   | -8.94 | 1.20        | 1.33     |
| 10  | C32   | 1671 | THR  | C-N   | -8.94 | 1.22        | 1.34     |
| 10  | C16   | 1447 | LEU  | C-N   | 8.93  | 1.46        | 1.33     |
| 20  | E8    | 430  | ALA  | C-N   | -8.93 | 1.20        | 1.33     |
| 10  | C16   | 716  | THR  | C-N   | 8.93  | 1.46        | 1.34     |
| 9   | K8    | 1216 | PRO  | N-CD  | -8.93 | 1.35        | 1.47     |
| 18  | B     | 1235 | PRO  | N-CD  | -8.93 | 1.35        | 1.47     |
| 10  | C     | 148  | GLU  | C-N   | -8.92 | 1.21        | 1.33     |
| 10  | C     | 358  | LYS  | C-N   | -8.92 | 1.21        | 1.33     |
| 18  | B     | 28   | LEU  | C-N   | 8.92  | 1.46        | 1.33     |
| 9   | K8    | 709  | MET  | C-N   | -8.92 | 1.22        | 1.33     |
| 10  | C32   | 148  | GLU  | C-N   | -8.92 | 1.21        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 833  | PRO  | N-CD  | -8.91 | 1.35        | 1.47     |
| 10  | C16   | 1131 | GLY  | C-N   | 8.90  | 1.45        | 1.33     |
| 10  | C24   | 148  | GLU  | C-N   | -8.90 | 1.21        | 1.33     |
| 18  | B8    | 689  | SER  | C-N   | 8.89  | 1.46        | 1.33     |
| 10  | C24   | 358  | LYS  | C-N   | -8.89 | 1.21        | 1.33     |
| 2   | M8    | 226  | LYS  | C-N   | -8.89 | 1.24        | 1.34     |
| 10  | C16   | 358  | LYS  | C-N   | -8.88 | 1.21        | 1.33     |
| 11  | A40   | 473  | GLY  | C-N   | 8.88  | 1.47        | 1.34     |
| 18  | B     | 294  | PHE  | C-N   | 8.88  | 1.46        | 1.34     |
| 18  | B8    | 517  | PRO  | N-CD  | -8.88 | 1.35        | 1.47     |
| 10  | C     | 1671 | THR  | C-N   | -8.87 | 1.22        | 1.34     |
| 20  | E     | 430  | ALA  | C-N   | -8.87 | 1.20        | 1.33     |
| 3   | N16   | 177  | TYR  | C-N   | 8.87  | 1.45        | 1.33     |
| 2   | M     | 226  | LYS  | C-N   | -8.87 | 1.24        | 1.34     |
| 11  | A24   | 850  | PRO  | N-CD  | -8.87 | 1.35        | 1.47     |
| 10  | C     | 56   | GLN  | C-N   | -8.87 | 1.23        | 1.34     |
| 11  | A16   | 847  | ARG  | C-N   | -8.86 | 1.22        | 1.33     |
| 12  | A     | 473  | GLY  | C-N   | 8.86  | 1.47        | 1.34     |
| 18  | B     | 74   | GLU  | C-N   | 8.86  | 1.45        | 1.33     |
| 10  | C32   | 1131 | GLY  | C-N   | 8.86  | 1.45        | 1.33     |
| 20  | E     | 431  | SER  | C-N   | 8.86  | 1.44        | 1.33     |
| 18  | B8    | 1235 | PRO  | N-CD  | -8.86 | 1.35        | 1.47     |
| 10  | C     | 1131 | GLY  | C-N   | 8.85  | 1.45        | 1.33     |
| 18  | B8    | 74   | GLU  | C-N   | 8.85  | 1.45        | 1.33     |
| 11  | A16   | 473  | GLY  | C-N   | 8.85  | 1.47        | 1.34     |
| 10  | C32   | 716  | THR  | C-N   | 8.85  | 1.46        | 1.34     |
| 18  | B     | 689  | SER  | C-N   | 8.84  | 1.46        | 1.33     |
| 11  | A24   | 847  | ARG  | C-N   | -8.84 | 1.22        | 1.33     |
| 20  | E8    | 431  | SER  | C-N   | 8.84  | 1.44        | 1.33     |
| 2   | M16   | 161  | ASP  | C-N   | -8.84 | 1.25        | 1.34     |
| 6   | O     | 240  | ARG  | C-N   | -8.84 | 1.26        | 1.33     |
| 9   | K8    | 1059 | ARG  | C-N   | -8.84 | 1.22        | 1.33     |
| 12  | A48   | 368  | THR  | C-N   | -8.84 | 1.22        | 1.33     |
| 18  | B8    | 1421 | ASN  | C-N   | 8.84  | 1.45        | 1.33     |
| 12  | A     | 368  | THR  | C-N   | -8.83 | 1.22        | 1.33     |
| 12  | A48   | 473  | GLY  | C-N   | 8.83  | 1.47        | 1.34     |
| 10  | C8    | 56   | GLN  | C-N   | -8.81 | 1.23        | 1.34     |
| 12  | A     | 847  | ARG  | C-N   | -8.81 | 1.22        | 1.33     |
| 18  | B8    | 72   | ILE  | C-N   | -8.81 | 1.21        | 1.33     |
| 3   | N     | 177  | TYR  | C-N   | 8.80  | 1.45        | 1.33     |
| 2   | M16   | 226  | LYS  | C-N   | -8.80 | 1.24        | 1.34     |
| 10  | C8    | 1131 | GLY  | C-N   | 8.80  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | N8    | 177  | TYR  | C-N   | 8.80  | 1.45        | 1.33     |
| 10  | C16   | 56   | GLN  | C-N   | -8.80 | 1.23        | 1.34     |
| 11  | A40   | 368  | THR  | C-N   | -8.80 | 1.22        | 1.33     |
| 12  | A48   | 847  | ARG  | C-N   | -8.80 | 1.22        | 1.33     |
| 5   | P8    | 162  | ALA  | C-N   | 8.80  | 1.45        | 1.33     |
| 5   | P     | 162  | ALA  | C-N   | 8.79  | 1.45        | 1.33     |
| 18  | B     | 517  | PRO  | N-CD  | -8.79 | 1.35        | 1.47     |
| 19  | 4     | 423  | PRO  | N-CD  | 8.79  | 1.60        | 1.47     |
| 18  | B     | 1421 | ASN  | C-N   | 8.79  | 1.45        | 1.33     |
| 11  | A16   | 368  | THR  | C-N   | -8.79 | 1.22        | 1.33     |
| 10  | C24   | 1131 | GLY  | C-N   | 8.78  | 1.45        | 1.33     |
| 10  | C     | 716  | THR  | C-N   | 8.78  | 1.46        | 1.34     |
| 11  | A32   | 368  | THR  | C-N   | -8.78 | 1.22        | 1.33     |
| 6   | O8    | 92   | ALA  | C-N   | 8.78  | 1.45        | 1.33     |
| 11  | A16   | 850  | PRO  | N-CD  | -8.78 | 1.35        | 1.47     |
| 10  | C24   | 56   | GLN  | C-N   | -8.78 | 1.23        | 1.34     |
| 11  | A32   | 473  | GLY  | C-N   | 8.78  | 1.47        | 1.34     |
| 5   | P16   | 162  | ALA  | C-N   | 8.77  | 1.45        | 1.33     |
| 10  | C32   | 1063 | PRO  | N-CD  | -8.77 | 1.35        | 1.47     |
| 2   | M16   | 344  | GLN  | C-N   | 8.77  | 1.44        | 1.33     |
| 10  | C     | 1063 | PRO  | N-CD  | -8.77 | 1.35        | 1.47     |
| 1   | R16   | 1242 | SER  | C-N   | -8.77 | 1.22        | 1.33     |
| 18  | B     | 72   | ILE  | C-N   | -8.76 | 1.21        | 1.33     |
| 11  | A40   | 850  | PRO  | N-CD  | -8.76 | 1.35        | 1.47     |
| 9   | K     | 1059 | ARG  | C-N   | -8.76 | 1.22        | 1.33     |
| 11  | A24   | 473  | GLY  | C-N   | 8.76  | 1.47        | 1.34     |
| 12  | A     | 850  | PRO  | N-CD  | -8.76 | 1.35        | 1.47     |
| 13  | V     | 786  | THR  | C-N   | -8.76 | 1.22        | 1.33     |
| 1   | R8    | 1242 | SER  | C-N   | -8.75 | 1.22        | 1.33     |
| 10  | C32   | 56   | GLN  | C-N   | -8.75 | 1.23        | 1.34     |
| 10  | C32   | 548  | ALA  | C-N   | 8.74  | 1.45        | 1.33     |
| 5   | P     | 715  | GLU  | C-N   | 8.74  | 1.45        | 1.33     |
| 19  | 48    | 423  | PRO  | N-CD  | 8.74  | 1.59        | 1.47     |
| 2   | M8    | 161  | ASP  | C-N   | -8.74 | 1.25        | 1.34     |
| 10  | C8    | 1063 | PRO  | N-CD  | -8.74 | 1.35        | 1.47     |
| 10  | C16   | 1063 | PRO  | N-CD  | -8.73 | 1.35        | 1.47     |
| 10  | C24   | 1063 | PRO  | N-CD  | -8.73 | 1.35        | 1.47     |
| 14  | W     | 698  | LEU  | C-N   | -8.73 | 1.22        | 1.34     |
| 11  | A32   | 847  | ARG  | C-N   | -8.73 | 1.22        | 1.33     |
| 2   | M8    | 344  | GLN  | C-N   | 8.72  | 1.44        | 1.33     |
| 6   | O8    | 240  | ARG  | C-N   | -8.72 | 1.26        | 1.33     |
| 5   | P8    | 715  | GLU  | C-N   | 8.72  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 1226 | GLY  | C-N   | 8.72  | 1.46        | 1.33     |
| 11  | A32   | 850  | PRO  | N-CD  | -8.72 | 1.35        | 1.47     |
| 10  | C     | 548  | ALA  | C-N   | 8.71  | 1.45        | 1.33     |
| 6   | O16   | 92   | ALA  | C-N   | 8.71  | 1.45        | 1.33     |
| 15  | J     | 671  | SER  | C-N   | -8.71 | 1.23        | 1.33     |
| 11  | A40   | 847  | ARG  | C-N   | -8.71 | 1.22        | 1.33     |
| 11  | A32   | 855  | GLU  | C-N   | -8.71 | 1.22        | 1.33     |
| 10  | C16   | 548  | ALA  | C-N   | 8.70  | 1.45        | 1.33     |
| 18  | B8    | 1226 | GLY  | C-N   | 8.70  | 1.46        | 1.33     |
| 10  | C24   | 548  | ALA  | C-N   | 8.70  | 1.45        | 1.33     |
| 11  | A24   | 368  | THR  | C-N   | -8.69 | 1.22        | 1.33     |
| 1   | R     | 1242 | SER  | C-N   | -8.68 | 1.22        | 1.33     |
| 18  | B     | 1146 | CYS  | C-N   | 8.68  | 1.45        | 1.33     |
| 18  | B     | 793  | LEU  | C-N   | 8.68  | 1.47        | 1.33     |
| 18  | B8    | 1146 | CYS  | C-N   | 8.68  | 1.45        | 1.33     |
| 13  | V     | 793  | GLU  | C-N   | -8.68 | 1.23        | 1.33     |
| 2   | M     | 344  | GLN  | C-N   | 8.67  | 1.44        | 1.33     |
| 10  | C8    | 548  | ALA  | C-N   | 8.67  | 1.45        | 1.33     |
| 10  | C32   | 660  | LEU  | C-N   | -8.67 | 1.22        | 1.33     |
| 11  | A40   | 855  | GLU  | C-N   | -8.67 | 1.22        | 1.33     |
| 11  | A24   | 855  | GLU  | C-N   | -8.67 | 1.22        | 1.33     |
| 2   | M     | 161  | ASP  | C-N   | -8.67 | 1.25        | 1.34     |
| 10  | C24   | 660  | LEU  | C-N   | -8.66 | 1.22        | 1.33     |
| 9   | K8    | 990  | PHE  | C-N   | -8.66 | 1.22        | 1.33     |
| 9   | K8    | 816  | HIS  | C-N   | -8.66 | 1.22        | 1.34     |
| 12  | A48   | 855  | GLU  | C-N   | -8.65 | 1.22        | 1.33     |
| 10  | C16   | 660  | LEU  | C-N   | -8.65 | 1.22        | 1.33     |
| 5   | P16   | 715  | GLU  | C-N   | 8.65  | 1.45        | 1.33     |
| 6   | O     | 92   | ALA  | C-N   | 8.65  | 1.44        | 1.33     |
| 12  | A48   | 850  | PRO  | N-CD  | -8.65 | 1.35        | 1.47     |
| 18  | B     | 688  | GLY  | C-N   | -8.64 | 1.21        | 1.33     |
| 15  | J     | 688  | PRO  | N-CD  | -8.64 | 1.35        | 1.47     |
| 7   | Q8    | 142  | TRP  | C-N   | -8.63 | 1.21        | 1.33     |
| 12  | A     | 855  | GLU  | C-N   | -8.63 | 1.22        | 1.33     |
| 11  | A16   | 855  | GLU  | C-N   | -8.63 | 1.22        | 1.33     |
| 18  | B8    | 793  | LEU  | C-N   | 8.63  | 1.47        | 1.33     |
| 20  | E     | 419  | ASN  | C-N   | -8.63 | 1.21        | 1.33     |
| 19  | 4     | 348  | SER  | C-N   | -8.62 | 1.21        | 1.33     |
| 2   | M16   | 621  | PHE  | C-N   | -8.62 | 1.21        | 1.33     |
| 7   | Q16   | 95   | PHE  | C-N   | 8.62  | 1.44        | 1.33     |
| 10  | C8    | 1710 | ASP  | C-N   | -8.62 | 1.23        | 1.33     |
| 20  | E8    | 419  | ASN  | C-N   | -8.62 | 1.21        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 1786 | LYS  | C-N   | -8.62 | 1.22        | 1.33     |
| 9   | K     | 816  | HIS  | C-N   | -8.62 | 1.22        | 1.34     |
| 2   | M8    | 621  | PHE  | C-N   | -8.61 | 1.21        | 1.33     |
| 7   | Q     | 142  | TRP  | C-N   | -8.60 | 1.21        | 1.33     |
| 7   | Q16   | 142  | TRP  | C-N   | -8.60 | 1.21        | 1.33     |
| 10  | C16   | 482  | MET  | C-N   | 8.60  | 1.45        | 1.33     |
| 10  | C8    | 482  | MET  | C-N   | 8.60  | 1.45        | 1.33     |
| 22  | I16   | 365  | ALA  | C-N   | 8.60  | 1.45        | 1.33     |
| 6   | O16   | 240  | ARG  | C-N   | -8.60 | 1.26        | 1.33     |
| 10  | C8    | 660  | LEU  | C-N   | -8.60 | 1.22        | 1.33     |
| 19  | 48    | 348  | SER  | C-N   | -8.60 | 1.21        | 1.33     |
| 2   | M     | 621  | PHE  | C-N   | -8.60 | 1.21        | 1.33     |
| 1   | R8    | 1248 | PRO  | C-N   | -8.59 | 1.21        | 1.33     |
| 22  | I24   | 365  | ALA  | C-N   | 8.59  | 1.45        | 1.33     |
| 7   | Q     | 219  | GLY  | C-N   | -8.59 | 1.21        | 1.33     |
| 10  | C32   | 482  | MET  | C-N   | 8.59  | 1.45        | 1.33     |
| 18  | B     | 1885 | SER  | C-N   | 8.59  | 1.46        | 1.33     |
| 10  | C32   | 1786 | LYS  | C-N   | -8.59 | 1.22        | 1.33     |
| 18  | B8    | 688  | GLY  | C-N   | -8.58 | 1.21        | 1.33     |
| 22  | I24   | 206  | PHE  | C-N   | 8.58  | 1.53        | 1.33     |
| 21  | H16   | 140  | PRO  | N-CD  | -8.58 | 1.35        | 1.47     |
| 10  | C     | 482  | MET  | C-N   | 8.57  | 1.45        | 1.33     |
| 10  | C     | 1786 | LYS  | C-N   | -8.57 | 1.22        | 1.33     |
| 18  | B8    | 1885 | SER  | C-N   | 8.57  | 1.46        | 1.33     |
| 18  | B     | 123  | LEU  | C-N   | -8.57 | 1.21        | 1.33     |
| 7   | Q     | 95   | PHE  | C-N   | 8.56  | 1.44        | 1.33     |
| 10  | C24   | 482  | MET  | C-N   | 8.56  | 1.45        | 1.33     |
| 14  | W     | 669  | LYS  | C-N   | -8.56 | 1.23        | 1.33     |
| 22  | I     | 206  | PHE  | C-N   | 8.56  | 1.53        | 1.33     |
| 1   | R16   | 1248 | PRO  | C-N   | -8.56 | 1.21        | 1.33     |
| 10  | C16   | 1702 | ASP  | C-N   | -8.56 | 1.23        | 1.34     |
| 1   | R     | 1248 | PRO  | C-N   | -8.56 | 1.21        | 1.33     |
| 22  | I8    | 206  | PHE  | C-N   | 8.56  | 1.53        | 1.33     |
| 21  | H24   | 140  | PRO  | N-CD  | -8.55 | 1.35        | 1.47     |
| 18  | B     | 318  | THR  | C-N   | 8.55  | 1.45        | 1.33     |
| 9   | K     | 990  | PHE  | C-N   | -8.55 | 1.22        | 1.33     |
| 7   | Q16   | 219  | GLY  | C-N   | -8.54 | 1.21        | 1.33     |
| 7   | Q8    | 219  | GLY  | C-N   | -8.54 | 1.21        | 1.33     |
| 5   | P8    | 614  | VAL  | C-N   | -8.54 | 1.21        | 1.33     |
| 6   | O16   | 18   | ASN  | C-N   | -8.54 | 1.22        | 1.33     |
| 10  | C     | 1702 | ASP  | C-N   | -8.54 | 1.23        | 1.34     |
| 22  | I16   | 206  | PHE  | C-N   | 8.54  | 1.53        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 1001 | LYS  | C-N   | -8.53 | 1.22        | 1.33     |
| 13  | V     | 880  | ARG  | C-N   | 8.53  | 1.46        | 1.33     |
| 21  | H     | 140  | PRO  | N-CD  | -8.53 | 1.35        | 1.47     |
| 22  | I8    | 365  | ALA  | C-N   | 8.53  | 1.45        | 1.33     |
| 3   | N8    | 146  | ASP  | C-N   | -8.52 | 1.21        | 1.33     |
| 20  | E     | 476  | PHE  | C-N   | -8.52 | 1.23        | 1.33     |
| 20  | E8    | 500  | PRO  | N-CD  | -8.52 | 1.35        | 1.47     |
| 21  | H8    | 140  | PRO  | N-CD  | -8.51 | 1.35        | 1.47     |
| 3   | N16   | 146  | ASP  | C-N   | -8.51 | 1.21        | 1.33     |
| 20  | E8    | 476  | PHE  | C-N   | -8.51 | 1.23        | 1.33     |
| 10  | C32   | 1710 | ASP  | C-N   | -8.51 | 1.23        | 1.33     |
| 10  | C24   | 1786 | LYS  | C-N   | -8.50 | 1.22        | 1.33     |
| 13  | V     | 883  | PRO  | N-CD  | -8.50 | 1.35        | 1.47     |
| 10  | C     | 660  | LEU  | C-N   | -8.50 | 1.22        | 1.33     |
| 11  | A16   | 56   | ALA  | C-N   | 8.49  | 1.53        | 1.33     |
| 20  | E     | 500  | PRO  | N-CD  | -8.48 | 1.35        | 1.47     |
| 10  | C8    | 1702 | ASP  | C-N   | -8.48 | 1.23        | 1.34     |
| 18  | B     | 1843 | THR  | C-N   | -8.48 | 1.22        | 1.33     |
| 5   | P8    | 591  | GLU  | C-N   | -8.48 | 1.21        | 1.33     |
| 15  | J     | 660  | HIS  | C-N   | -8.48 | 1.22        | 1.34     |
| 18  | B8    | 318  | THR  | C-N   | 8.48  | 1.45        | 1.33     |
| 18  | B8    | 123  | LEU  | C-N   | -8.47 | 1.21        | 1.33     |
| 6   | O8    | 18   | ASN  | C-N   | -8.47 | 1.22        | 1.33     |
| 5   | P16   | 591  | GLU  | C-N   | -8.47 | 1.22        | 1.33     |
| 22  | I     | 367  | ARG  | C-N   | -8.47 | 1.23        | 1.33     |
| 18  | B8    | 1843 | THR  | C-N   | -8.47 | 1.22        | 1.33     |
| 22  | I     | 365  | ALA  | C-N   | 8.47  | 1.45        | 1.33     |
| 5   | P     | 591  | GLU  | C-N   | -8.47 | 1.22        | 1.33     |
| 11  | A32   | 56   | ALA  | C-N   | 8.47  | 1.53        | 1.33     |
| 3   | N16   | 45   | GLY  | C-N   | 8.46  | 1.44        | 1.33     |
| 9   | K8    | 1001 | LYS  | C-N   | -8.46 | 1.22        | 1.33     |
| 10  | C     | 1710 | ASP  | C-N   | -8.46 | 1.23        | 1.33     |
| 11  | A16   | 744  | GLU  | C-N   | -8.45 | 1.22        | 1.34     |
| 10  | C32   | 1702 | ASP  | C-N   | -8.46 | 1.23        | 1.34     |
| 3   | N8    | 45   | GLY  | C-N   | 8.45  | 1.44        | 1.33     |
| 11  | A40   | 56   | ALA  | C-N   | 8.45  | 1.53        | 1.33     |
| 10  | C8    | 1786 | LYS  | C-N   | -8.45 | 1.22        | 1.33     |
| 19  | 48    | 344  | PRO  | N-CD  | -8.45 | 1.35        | 1.47     |
| 10  | C16   | 1710 | ASP  | C-N   | -8.44 | 1.23        | 1.33     |
| 1   | R8    | 1156 | GLU  | C-N   | -8.44 | 1.23        | 1.33     |
| 10  | C24   | 43   | LEU  | C-N   | -8.44 | 1.21        | 1.33     |
| 3   | N     | 146  | ASP  | C-N   | -8.44 | 1.21        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 1017 | LEU  | C-N   | -8.44 | 1.22        | 1.34     |
| 10  | C     | 1759 | ALA  | C-N   | -8.44 | 1.22        | 1.33     |
| 6   | O     | 18   | ASN  | C-N   | -8.44 | 1.22        | 1.33     |
| 11  | A24   | 744  | GLU  | C-N   | -8.44 | 1.22        | 1.34     |
| 11  | A24   | 56   | ALA  | C-N   | 8.43  | 1.53        | 1.33     |
| 10  | C8    | 1636 | ARG  | C-N   | -8.43 | 1.22        | 1.33     |
| 10  | C32   | 1542 | PHE  | C-N   | 8.43  | 1.45        | 1.33     |
| 2   | M     | 193  | PRO  | N-CD  | -8.43 | 1.35        | 1.47     |
| 10  | C24   | 1702 | ASP  | C-N   | -8.43 | 1.23        | 1.34     |
| 10  | C     | 112  | PRO  | N-CD  | -8.43 | 1.35        | 1.47     |
| 20  | E8    | 490  | GLY  | C-N   | -8.42 | 1.22        | 1.33     |
| 22  | I24   | 367  | ARG  | C-N   | -8.42 | 1.23        | 1.33     |
| 22  | I8    | 159  | ARG  | C-N   | -8.42 | 1.23        | 1.33     |
| 10  | C24   | 112  | PRO  | N-CD  | -8.42 | 1.35        | 1.47     |
| 22  | I     | 159  | ARG  | C-N   | -8.42 | 1.23        | 1.33     |
| 19  | 4     | 344  | PRO  | N-CD  | -8.41 | 1.35        | 1.47     |
| 10  | C32   | 43   | LEU  | C-N   | -8.41 | 1.21        | 1.33     |
| 10  | C16   | 1542 | PHE  | C-N   | 8.41  | 1.45        | 1.33     |
| 10  | C32   | 112  | PRO  | N-CD  | -8.41 | 1.35        | 1.47     |
| 22  | I24   | 159  | ARG  | C-N   | -8.41 | 1.23        | 1.33     |
| 22  | I8    | 367  | ARG  | C-N   | -8.40 | 1.23        | 1.33     |
| 1   | R     | 1156 | GLU  | C-N   | -8.40 | 1.23        | 1.33     |
| 20  | E     | 490  | GLY  | C-N   | -8.40 | 1.22        | 1.33     |
| 10  | C16   | 43   | LEU  | C-N   | -8.39 | 1.21        | 1.33     |
| 3   | N     | 45   | GLY  | C-N   | 8.39  | 1.44        | 1.33     |
| 10  | C16   | 112  | PRO  | N-CD  | -8.38 | 1.36        | 1.47     |
| 10  | C16   | 1636 | ARG  | C-N   | -8.38 | 1.22        | 1.33     |
| 18  | B8    | 984  | LYS  | C-N   | 8.38  | 1.45        | 1.33     |
| 22  | I16   | 159  | ARG  | C-N   | -8.38 | 1.23        | 1.33     |
| 10  | C16   | 1055 | GLU  | C-N   | -8.37 | 1.22        | 1.33     |
| 9   | K8    | 1017 | LEU  | C-N   | -8.37 | 1.22        | 1.34     |
| 10  | C24   | 1636 | ARG  | C-N   | -8.37 | 1.22        | 1.33     |
| 18  | B     | 917  | PHE  | C-N   | 8.37  | 1.45        | 1.33     |
| 10  | C     | 1636 | ARG  | C-N   | -8.37 | 1.22        | 1.33     |
| 10  | C8    | 43   | LEU  | C-N   | -8.36 | 1.22        | 1.33     |
| 12  | A     | 744  | GLU  | C-N   | -8.35 | 1.22        | 1.34     |
| 9   | K     | 1250 | SER  | C-N   | -8.35 | 1.22        | 1.33     |
| 10  | C24   | 1710 | ASP  | C-N   | -8.35 | 1.23        | 1.33     |
| 22  | I16   | 367  | ARG  | C-N   | -8.35 | 1.23        | 1.33     |
| 10  | C16   | 21   | PRO  | N-CD  | -8.35 | 1.36        | 1.47     |
| 10  | C32   | 1636 | ARG  | C-N   | -8.35 | 1.22        | 1.33     |
| 2   | M8    | 193  | PRO  | N-CD  | -8.34 | 1.36        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | P8    | 206  | SER  | C-N   | 8.34  | 1.42        | 1.33     |
| 10  | C24   | 1542 | PHE  | C-N   | 8.34  | 1.45        | 1.33     |
| 15  | J     | 600  | GLU  | C-N   | -8.34 | 1.22        | 1.33     |
| 10  | C8    | 112  | PRO  | N-CD  | -8.34 | 1.36        | 1.47     |
| 11  | A32   | 744  | GLU  | C-N   | -8.34 | 1.22        | 1.34     |
| 5   | P     | 206  | SER  | C-N   | 8.34  | 1.42        | 1.33     |
| 19  | 4     | 116  | PHE  | C-N   | -8.34 | 1.23        | 1.33     |
| 10  | C32   | 1055 | GLU  | C-N   | -8.33 | 1.22        | 1.33     |
| 10  | C16   | 1759 | ALA  | C-N   | -8.33 | 1.23        | 1.33     |
| 18  | B8    | 911  | ILE  | C-N   | 8.33  | 1.44        | 1.33     |
| 18  | B8    | 969  | ASP  | C-N   | 8.33  | 1.44        | 1.33     |
| 11  | A40   | 744  | GLU  | C-N   | -8.32 | 1.22        | 1.34     |
| 18  | B8    | 1672 | ASP  | C-N   | 8.32  | 1.43        | 1.33     |
| 10  | C     | 43   | LEU  | C-N   | -8.32 | 1.22        | 1.33     |
| 12  | A48   | 744  | GLU  | C-N   | -8.32 | 1.22        | 1.34     |
| 10  | C8    | 1542 | PHE  | C-N   | 8.32  | 1.45        | 1.33     |
| 14  | W     | 631  | TYR  | C-N   | -8.32 | 1.24        | 1.33     |
| 18  | B     | 911  | ILE  | C-N   | 8.32  | 1.44        | 1.33     |
| 10  | C24   | 1759 | ALA  | C-N   | -8.32 | 1.23        | 1.33     |
| 1   | R     | 1379 | GLN  | C-N   | -8.31 | 1.23        | 1.33     |
| 10  | C32   | 1759 | ALA  | C-N   | -8.31 | 1.23        | 1.33     |
| 2   | M16   | 193  | PRO  | N-CD  | -8.31 | 1.36        | 1.47     |
| 18  | B8    | 1377 | ASP  | C-N   | -8.31 | 1.22        | 1.33     |
| 1   | R8    | 1379 | GLN  | C-N   | -8.31 | 1.23        | 1.33     |
| 5   | P16   | 206  | SER  | C-N   | 8.30  | 1.42        | 1.33     |
| 9   | K8    | 1250 | SER  | C-N   | -8.30 | 1.22        | 1.33     |
| 10  | C24   | 1055 | GLU  | C-N   | -8.29 | 1.22        | 1.33     |
| 1   | R16   | 1156 | GLU  | C-N   | -8.29 | 1.23        | 1.33     |
| 10  | C     | 1055 | GLU  | C-N   | -8.29 | 1.22        | 1.33     |
| 1   | R16   | 1289 | ALA  | C-N   | -8.29 | 1.24        | 1.33     |
| 9   | K8    | 1118 | PRO  | C-N   | 8.29  | 1.44        | 1.33     |
| 18  | B     | 1377 | ASP  | C-N   | -8.28 | 1.22        | 1.33     |
| 5   | P16   | 359  | TRP  | C-N   | 8.28  | 1.44        | 1.33     |
| 18  | B8    | 917  | PHE  | C-N   | 8.28  | 1.45        | 1.33     |
| 10  | C8    | 21   | PRO  | N-CD  | -8.28 | 1.36        | 1.47     |
| 19  | 48    | 116  | PHE  | C-N   | -8.28 | 1.23        | 1.33     |
| 18  | B     | 969  | ASP  | C-N   | 8.27  | 1.44        | 1.33     |
| 19  | 4     | 35   | GLY  | C-N   | -8.27 | 1.22        | 1.34     |
| 19  | 48    | 35   | GLY  | C-N   | -8.27 | 1.22        | 1.34     |
| 10  | C8    | 1759 | ALA  | C-N   | -8.27 | 1.23        | 1.33     |
| 18  | B     | 1672 | ASP  | C-N   | 8.26  | 1.43        | 1.33     |
| 6   | O8    | 278  | GLY  | C-N   | -8.26 | 1.21        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 21   | PRO  | N-CD  | -8.26 | 1.36        | 1.47     |
| 10  | C8    | 1055 | GLU  | C-N   | -8.26 | 1.22        | 1.33     |
| 9   | K8    | 1169 | GLU  | C-N   | -8.25 | 1.22        | 1.34     |
| 9   | K     | 1118 | PRO  | C-N   | 8.25  | 1.44        | 1.33     |
| 10  | C     | 21   | PRO  | N-CD  | -8.24 | 1.36        | 1.47     |
| 1   | R8    | 1452 | GLU  | C-N   | -8.24 | 1.23        | 1.33     |
| 11  | A24   | 26   | PRO  | C-N   | 8.24  | 1.45        | 1.33     |
| 13  | V     | 814  | MET  | C-N   | -8.24 | 1.23        | 1.33     |
| 9   | K     | 1169 | GLU  | C-N   | -8.24 | 1.22        | 1.34     |
| 9   | K8    | 1117 | LEU  | C-N   | 8.23  | 1.45        | 1.33     |
| 11  | A16   | 26   | PRO  | C-N   | 8.23  | 1.45        | 1.33     |
| 1   | R8    | 1289 | ALA  | C-N   | -8.23 | 1.24        | 1.33     |
| 9   | K     | 833  | THR  | C-N   | -8.22 | 1.23        | 1.33     |
| 10  | C8    | 1311 | GLU  | C-N   | 8.22  | 1.44        | 1.33     |
| 18  | B8    | 1113 | PRO  | C-N   | -8.22 | 1.23        | 1.33     |
| 2   | M16   | 331  | LEU  | C-N   | 8.22  | 1.44        | 1.33     |
| 5   | P8    | 359  | TRP  | C-N   | 8.21  | 1.44        | 1.33     |
| 18  | B     | 984  | LYS  | C-N   | 8.21  | 1.45        | 1.33     |
| 5   | P     | 189  | PRO  | N-CD  | 8.21  | 1.59        | 1.47     |
| 6   | O16   | 278  | GLY  | C-N   | -8.21 | 1.22        | 1.33     |
| 11  | A40   | 26   | PRO  | C-N   | 8.21  | 1.45        | 1.33     |
| 11  | A32   | 26   | PRO  | C-N   | 8.20  | 1.45        | 1.33     |
| 10  | C24   | 846  | LEU  | C-N   | -8.20 | 1.22        | 1.33     |
| 5   | P     | 359  | TRP  | C-N   | 8.20  | 1.44        | 1.33     |
| 5   | P8    | 669  | ASN  | C-N   | -8.20 | 1.23        | 1.33     |
| 5   | P     | 669  | ASN  | C-N   | -8.19 | 1.23        | 1.33     |
| 9   | K     | 1259 | LYS  | C-N   | -8.19 | 1.22        | 1.33     |
| 1   | R16   | 1379 | GLN  | C-N   | -8.19 | 1.23        | 1.33     |
| 9   | K8    | 624  | ALA  | C-N   | -8.19 | 1.22        | 1.33     |
| 1   | R     | 1452 | GLU  | C-N   | -8.18 | 1.23        | 1.33     |
| 22  | I24   | 347  | HIS  | C-N   | 8.18  | 1.50        | 1.33     |
| 5   | P8    | 189  | PRO  | N-CD  | 8.17  | 1.59        | 1.47     |
| 2   | M     | 331  | LEU  | C-N   | 8.17  | 1.44        | 1.33     |
| 11  | A24   | 157  | LEU  | C-N   | 8.17  | 1.52        | 1.33     |
| 10  | C8    | 177  | GLU  | C-N   | -8.17 | 1.22        | 1.33     |
| 10  | C8    | 1789 | ILE  | C-N   | 8.17  | 1.45        | 1.34     |
| 2   | M8    | 331  | LEU  | C-N   | 8.17  | 1.44        | 1.33     |
| 10  | C     | 1311 | GLU  | C-N   | 8.17  | 1.44        | 1.33     |
| 10  | C16   | 846  | LEU  | C-N   | -8.17 | 1.22        | 1.33     |
| 10  | C24   | 1789 | ILE  | C-N   | 8.17  | 1.45        | 1.34     |
| 6   | O     | 278  | GLY  | C-N   | -8.16 | 1.22        | 1.33     |
| 22  | I16   | 347  | HIS  | C-N   | 8.16  | 1.50        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 19  | 4     | 359  | ALA  | C-N   | -8.16 | 1.22        | 1.33     |
| 19  | 48    | 310  | ARG  | C-N   | -8.16 | 1.23        | 1.33     |
| 22  | I8    | 347  | HIS  | C-N   | 8.16  | 1.50        | 1.33     |
| 9   | K     | 1046 | LEU  | C-N   | -8.16 | 1.22        | 1.33     |
| 11  | A40   | 157  | LEU  | C-N   | 8.15  | 1.52        | 1.33     |
| 10  | C32   | 21   | PRO  | N-CD  | -8.15 | 1.36        | 1.47     |
| 10  | C24   | 177  | GLU  | C-N   | -8.15 | 1.22        | 1.33     |
| 12  | A     | 157  | LEU  | C-N   | 8.15  | 1.52        | 1.33     |
| 9   | K8    | 833  | THR  | C-N   | -8.14 | 1.23        | 1.33     |
| 22  | I     | 347  | HIS  | C-N   | 8.14  | 1.50        | 1.33     |
| 7   | Q16   | 78   | SER  | C-N   | -8.13 | 1.22        | 1.33     |
| 19  | 48    | 359  | ALA  | C-N   | -8.14 | 1.22        | 1.33     |
| 10  | C     | 951  | PRO  | N-CD  | -8.13 | 1.36        | 1.47     |
| 16  | A8    | 157  | LEU  | C-N   | 8.13  | 1.52        | 1.33     |
| 1   | R16   | 1452 | GLU  | C-N   | -8.13 | 1.23        | 1.33     |
| 18  | B     | 1747 | SER  | C-N   | 8.13  | 1.47        | 1.33     |
| 19  | 4     | 98   | SER  | C-N   | -8.13 | 1.21        | 1.33     |
| 12  | A48   | 157  | LEU  | C-N   | 8.13  | 1.52        | 1.33     |
| 1   | R     | 1289 | ALA  | C-N   | -8.13 | 1.24        | 1.33     |
| 19  | 48    | 92   | THR  | C-N   | -8.13 | 1.22        | 1.33     |
| 19  | 48    | 98   | SER  | C-N   | -8.12 | 1.21        | 1.33     |
| 9   | K8    | 1046 | LEU  | C-N   | -8.12 | 1.22        | 1.33     |
| 9   | K     | 1117 | LEU  | C-N   | 8.12  | 1.45        | 1.33     |
| 10  | C16   | 1311 | GLU  | C-N   | 8.12  | 1.44        | 1.33     |
| 19  | 4     | 92   | THR  | C-N   | -8.12 | 1.22        | 1.33     |
| 10  | C32   | 846  | LEU  | C-N   | -8.12 | 1.22        | 1.33     |
| 7   | Q8    | 78   | SER  | C-N   | -8.12 | 1.22        | 1.33     |
| 9   | K8    | 1259 | LYS  | C-N   | -8.11 | 1.22        | 1.33     |
| 10  | C24   | 1311 | GLU  | C-N   | 8.11  | 1.44        | 1.33     |
| 10  | C     | 1789 | ILE  | C-N   | 8.11  | 1.44        | 1.34     |
| 10  | C8    | 951  | PRO  | N-CD  | -8.11 | 1.36        | 1.47     |
| 18  | B     | 918  | GLY  | C-N   | 8.11  | 1.44        | 1.33     |
| 2   | M     | 528  | PHE  | C-N   | 8.10  | 1.45        | 1.33     |
| 18  | B8    | 918  | GLY  | C-N   | 8.10  | 1.44        | 1.33     |
| 9   | K     | 624  | ALA  | C-N   | -8.10 | 1.23        | 1.33     |
| 18  | B     | 1684 | TRP  | C-N   | 8.10  | 1.45        | 1.33     |
| 10  | C16   | 1789 | ILE  | C-N   | 8.09  | 1.44        | 1.34     |
| 7   | Q8    | 31   | LEU  | C-N   | -8.09 | 1.22        | 1.33     |
| 18  | B     | 1665 | ALA  | C-N   | -8.09 | 1.23        | 1.33     |
| 20  | E     | 306  | SER  | C-N   | -8.09 | 1.23        | 1.33     |
| 9   | K8    | 783  | ARG  | C-N   | -8.09 | 1.22        | 1.33     |
| 5   | P16   | 189  | PRO  | N-CD  | 8.08  | 1.59        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C8    | 846  | LEU  | C-N   | -8.08 | 1.22        | 1.33     |
| 10  | C32   | 1311 | GLU  | C-N   | 8.08  | 1.44        | 1.33     |
| 7   | Q     | 78   | SER  | C-N   | -8.08 | 1.22        | 1.33     |
| 10  | C32   | 1535 | LEU  | C-N   | 8.07  | 1.41        | 1.33     |
| 18  | B8    | 1665 | ALA  | C-N   | -8.07 | 1.23        | 1.33     |
| 18  | B     | 1113 | PRO  | C-N   | -8.07 | 1.23        | 1.33     |
| 19  | 4     | 310  | ARG  | C-N   | -8.07 | 1.23        | 1.33     |
| 10  | C     | 846  | LEU  | C-N   | -8.07 | 1.22        | 1.33     |
| 10  | C32   | 951  | PRO  | N-CD  | -8.07 | 1.36        | 1.47     |
| 10  | C16   | 1439 | ILE  | C-N   | 8.06  | 1.45        | 1.33     |
| 5   | P16   | 669  | ASN  | C-N   | -8.06 | 1.23        | 1.33     |
| 10  | C16   | 1734 | ARG  | C-N   | -8.06 | 1.23        | 1.33     |
| 10  | C32   | 1734 | ARG  | C-N   | -8.06 | 1.23        | 1.33     |
| 18  | B8    | 1747 | SER  | C-N   | 8.06  | 1.46        | 1.33     |
| 2   | M     | 445  | ASN  | C-N   | -8.05 | 1.23        | 1.33     |
| 7   | Q     | 31   | LEU  | C-N   | -8.05 | 1.22        | 1.33     |
| 10  | C8    | 653  | TYR  | C-N   | -8.05 | 1.23        | 1.34     |
| 9   | K     | 783  | ARG  | C-N   | -8.05 | 1.22        | 1.33     |
| 2   | M8    | 528  | PHE  | C-N   | 8.05  | 1.45        | 1.33     |
| 2   | M16   | 445  | ASN  | C-N   | -8.04 | 1.23        | 1.33     |
| 10  | C8    | 1535 | LEU  | C-N   | 8.04  | 1.41        | 1.33     |
| 20  | E8    | 37   | LEU  | C-N   | 8.04  | 1.44        | 1.33     |
| 9   | K     | 1212 | ARG  | C-N   | -8.04 | 1.22        | 1.33     |
| 10  | C8    | 1439 | ILE  | C-N   | 8.04  | 1.45        | 1.33     |
| 20  | E8    | 306  | SER  | C-N   | -8.04 | 1.23        | 1.33     |
| 10  | C16   | 1535 | LEU  | C-N   | 8.03  | 1.41        | 1.33     |
| 2   | M8    | 445  | ASN  | C-N   | -8.02 | 1.23        | 1.33     |
| 10  | C     | 1439 | ILE  | C-N   | 8.02  | 1.44        | 1.33     |
| 10  | C8    | 437  | ARG  | C-N   | -8.02 | 1.24        | 1.33     |
| 18  | B8    | 1684 | TRP  | C-N   | 8.02  | 1.45        | 1.33     |
| 20  | E     | 37   | LEU  | C-N   | 8.02  | 1.44        | 1.33     |
| 10  | C32   | 1439 | ILE  | C-N   | 8.02  | 1.45        | 1.33     |
| 6   | O16   | 237  | ASN  | C-N   | -8.02 | 1.25        | 1.33     |
| 10  | C24   | 1439 | ILE  | C-N   | 8.02  | 1.44        | 1.33     |
| 10  | C     | 437  | ARG  | C-N   | -8.02 | 1.24        | 1.33     |
| 10  | C32   | 177  | GLU  | C-N   | -8.01 | 1.22        | 1.33     |
| 10  | C24   | 1734 | ARG  | C-N   | -8.01 | 1.23        | 1.33     |
| 18  | B     | 509  | SER  | C-N   | 8.01  | 1.45        | 1.33     |
| 18  | B     | 968  | PHE  | C-N   | 8.01  | 1.44        | 1.33     |
| 10  | C     | 177  | GLU  | C-N   | -8.01 | 1.22        | 1.33     |
| 7   | Q16   | 31   | LEU  | C-N   | -8.00 | 1.22        | 1.33     |
| 10  | C24   | 437  | ARG  | C-N   | -8.00 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1535 | LEU  | C-N   | 7.99  | 1.41        | 1.33     |
| 10  | C32   | 1789 | ILE  | C-N   | 7.99  | 1.44        | 1.34     |
| 2   | M16   | 528  | PHE  | C-N   | 7.99  | 1.45        | 1.33     |
| 10  | C8    | 1734 | ARG  | C-N   | -7.99 | 1.23        | 1.33     |
| 2   | M8    | 458  | LYS  | C-N   | -7.99 | 1.23        | 1.33     |
| 10  | C     | 1535 | LEU  | C-N   | 7.99  | 1.41        | 1.33     |
| 18  | B8    | 968  | PHE  | C-N   | 7.99  | 1.44        | 1.33     |
| 22  | I     | 323  | GLU  | C-N   | -7.99 | 1.23        | 1.33     |
| 3   | N16   | 254  | VAL  | C-N   | -7.98 | 1.23        | 1.33     |
| 18  | B8    | 1539 | LEU  | C-N   | -7.98 | 1.23        | 1.33     |
| 2   | M     | 458  | LYS  | C-N   | -7.98 | 1.23        | 1.33     |
| 2   | M16   | 765  | THR  | C-N   | -7.98 | 1.23        | 1.33     |
| 10  | C16   | 951  | PRO  | N-CD  | -7.98 | 1.36        | 1.47     |
| 10  | C24   | 106  | GLY  | C-N   | -7.98 | 1.21        | 1.33     |
| 22  | I16   | 323  | GLU  | C-N   | -7.98 | 1.23        | 1.33     |
| 2   | M16   | 750  | GLN  | C-N   | 7.97  | 1.44        | 1.33     |
| 10  | C16   | 177  | GLU  | C-N   | -7.97 | 1.22        | 1.33     |
| 10  | C32   | 1281 | THR  | C-N   | -7.97 | 1.23        | 1.34     |
| 10  | C24   | 951  | PRO  | N-CD  | -7.97 | 1.36        | 1.47     |
| 10  | C     | 653  | TYR  | C-N   | -7.97 | 1.23        | 1.34     |
| 6   | O     | 185  | PRO  | C-N   | -7.96 | 1.21        | 1.33     |
| 14  | W     | 676  | PHE  | C-N   | -7.96 | 1.23        | 1.33     |
| 10  | C     | 1277 | SER  | C-N   | -7.96 | 1.22        | 1.33     |
| 6   | O8    | 237  | ASN  | C-N   | -7.96 | 1.25        | 1.33     |
| 9   | K8    | 1212 | ARG  | C-N   | -7.95 | 1.22        | 1.33     |
| 10  | C16   | 437  | ARG  | C-N   | -7.95 | 1.24        | 1.33     |
| 10  | C     | 465  | PHE  | C-N   | -7.95 | 1.23        | 1.34     |
| 18  | B8    | 194  | ASN  | C-N   | 7.95  | 1.44        | 1.33     |
| 9   | K     | 1165 | SER  | C-N   | -7.95 | 1.23        | 1.34     |
| 10  | C32   | 653  | TYR  | C-N   | -7.95 | 1.23        | 1.34     |
| 18  | B8    | 509  | SER  | C-N   | 7.94  | 1.45        | 1.33     |
| 18  | B     | 409  | LEU  | C-N   | 7.94  | 1.44        | 1.33     |
| 2   | M16   | 458  | LYS  | C-N   | -7.94 | 1.23        | 1.33     |
| 6   | O8    | 185  | PRO  | C-N   | -7.94 | 1.21        | 1.33     |
| 22  | I24   | 323  | GLU  | C-N   | -7.94 | 1.23        | 1.33     |
| 10  | C24   | 878  | ARG  | C-N   | -7.94 | 1.23        | 1.34     |
| 10  | C     | 878  | ARG  | C-N   | -7.94 | 1.23        | 1.34     |
| 10  | C8    | 106  | GLY  | C-N   | -7.94 | 1.21        | 1.33     |
| 10  | C8    | 465  | PHE  | C-N   | -7.94 | 1.23        | 1.34     |
| 2   | M8    | 750  | GLN  | C-N   | 7.93  | 1.44        | 1.33     |
| 21  | H16   | 162  | LYS  | C-N   | -7.93 | 1.23        | 1.33     |
| 10  | C16   | 653  | TYR  | C-N   | -7.93 | 1.23        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1277 | SER  | C-N   | -7.93 | 1.22        | 1.33     |
| 18  | B     | 1539 | LEU  | C-N   | -7.93 | 1.23        | 1.33     |
| 18  | B8    | 825  | ALA  | C-N   | 7.93  | 1.44        | 1.33     |
| 18  | B     | 825  | ALA  | C-N   | 7.92  | 1.44        | 1.33     |
| 17  | F16   | 65   | ARG  | C-N   | -7.92 | 1.23        | 1.34     |
| 10  | C8    | 287  | SER  | C-N   | 7.92  | 1.45        | 1.33     |
| 3   | N8    | 254  | VAL  | C-N   | -7.92 | 1.23        | 1.33     |
| 2   | M     | 750  | GLN  | C-N   | 7.92  | 1.44        | 1.33     |
| 18  | B     | 1603 | ASP  | C-N   | 7.92  | 1.44        | 1.33     |
| 18  | B8    | 958  | ARG  | C-N   | 7.92  | 1.46        | 1.33     |
| 21  | H8    | 162  | LYS  | C-N   | -7.92 | 1.23        | 1.33     |
| 10  | C32   | 437  | ARG  | C-N   | -7.92 | 1.24        | 1.33     |
| 3   | N     | 254  | VAL  | C-N   | -7.91 | 1.23        | 1.33     |
| 6   | O     | 237  | ASN  | C-N   | -7.91 | 1.25        | 1.33     |
| 10  | C16   | 1277 | SER  | C-N   | -7.91 | 1.22        | 1.33     |
| 18  | B8    | 1603 | ASP  | C-N   | 7.91  | 1.44        | 1.33     |
| 9   | K8    | 1026 | LEU  | C-N   | -7.91 | 1.23        | 1.33     |
| 10  | C     | 287  | SER  | C-N   | 7.91  | 1.45        | 1.33     |
| 9   | K8    | 1165 | SER  | C-N   | -7.91 | 1.23        | 1.34     |
| 9   | K8    | 1263 | THR  | C-N   | -7.91 | 1.23        | 1.33     |
| 10  | C     | 106  | GLY  | C-N   | -7.91 | 1.21        | 1.33     |
| 17  | F24   | 65   | ARG  | C-N   | -7.91 | 1.23        | 1.34     |
| 18  | B8    | 409  | LEU  | C-N   | 7.91  | 1.44        | 1.33     |
| 20  | E8    | 349  | THR  | C-N   | 7.91  | 1.44        | 1.33     |
| 10  | C32   | 465  | PHE  | C-N   | -7.91 | 1.23        | 1.34     |
| 10  | C     | 1734 | ARG  | C-N   | -7.90 | 1.23        | 1.33     |
| 10  | C8    | 1281 | THR  | C-N   | -7.90 | 1.23        | 1.34     |
| 10  | C32   | 1277 | SER  | C-N   | -7.90 | 1.22        | 1.33     |
| 10  | C16   | 287  | SER  | C-N   | 7.90  | 1.45        | 1.33     |
| 10  | C16   | 878  | ARG  | C-N   | -7.90 | 1.23        | 1.34     |
| 10  | C24   | 471  | THR  | C-N   | -7.89 | 1.21        | 1.33     |
| 14  | W     | 801  | ALA  | C-N   | -7.89 | 1.23        | 1.33     |
| 21  | H     | 162  | LYS  | C-N   | -7.89 | 1.23        | 1.33     |
| 10  | C24   | 465  | PHE  | C-N   | -7.89 | 1.23        | 1.34     |
| 18  | B     | 194  | ASN  | C-N   | 7.89  | 1.43        | 1.33     |
| 10  | C32   | 287  | SER  | C-N   | 7.88  | 1.45        | 1.33     |
| 10  | C     | 1281 | THR  | C-N   | -7.88 | 1.23        | 1.34     |
| 10  | C24   | 653  | TYR  | C-N   | -7.88 | 1.23        | 1.34     |
| 13  | V     | 788  | HIS  | C-N   | -7.88 | 1.23        | 1.33     |
| 22  | I24   | 252  | ARG  | C-N   | 7.88  | 1.44        | 1.33     |
| 20  | E8    | 462  | THR  | C-N   | -7.88 | 1.23        | 1.33     |
| 10  | C24   | 287  | SER  | C-N   | 7.87  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | I     | 252  | ARG  | C-N   | 7.87  | 1.44        | 1.33     |
| 10  | C16   | 106  | GLY  | C-N   | -7.87 | 1.21        | 1.33     |
| 10  | C16   | 465  | PHE  | C-N   | -7.87 | 1.23        | 1.34     |
| 22  | I8    | 252  | ARG  | C-N   | 7.87  | 1.44        | 1.33     |
| 22  | I8    | 323  | GLU  | C-N   | -7.87 | 1.23        | 1.33     |
| 10  | C16   | 471  | THR  | C-N   | -7.87 | 1.21        | 1.33     |
| 14  | W     | 665  | GLU  | C-N   | -7.87 | 1.23        | 1.33     |
| 10  | C16   | 1281 | THR  | C-N   | -7.86 | 1.23        | 1.34     |
| 10  | C24   | 1281 | THR  | C-N   | -7.86 | 1.23        | 1.34     |
| 1   | R16   | 1432 | LYS  | C-N   | -7.86 | 1.22        | 1.33     |
| 10  | C8    | 878  | ARG  | C-N   | -7.86 | 1.23        | 1.34     |
| 6   | O16   | 185  | PRO  | C-N   | -7.86 | 1.21        | 1.33     |
| 10  | C32   | 471  | THR  | C-N   | -7.86 | 1.21        | 1.33     |
| 11  | A32   | 155  | SER  | C-N   | 7.86  | 1.44        | 1.33     |
| 13  | V     | 753  | GLY  | C-N   | -7.85 | 1.23        | 1.34     |
| 10  | C     | 1792 | GLU  | C-N   | -7.85 | 1.24        | 1.33     |
| 13  | V     | 806  | ALA  | C-N   | -7.85 | 1.23        | 1.33     |
| 9   | K     | 1026 | LEU  | C-N   | -7.85 | 1.23        | 1.33     |
| 21  | H24   | 162  | LYS  | C-N   | -7.85 | 1.23        | 1.33     |
| 22  | I16   | 252  | ARG  | C-N   | 7.85  | 1.44        | 1.33     |
| 10  | C     | 760  | GLY  | C-N   | -7.85 | 1.24        | 1.33     |
| 10  | C32   | 878  | ARG  | C-N   | -7.84 | 1.23        | 1.34     |
| 9   | K     | 1263 | THR  | C-N   | -7.84 | 1.23        | 1.33     |
| 9   | K     | 656  | LEU  | C-N   | -7.84 | 1.24        | 1.33     |
| 2   | M     | 765  | THR  | C-N   | -7.84 | 1.23        | 1.33     |
| 2   | M8    | 765  | THR  | C-N   | -7.84 | 1.23        | 1.33     |
| 9   | K     | 1076 | ARG  | C-N   | -7.84 | 1.23        | 1.33     |
| 19  | 48    | 169  | CYS  | C-N   | -7.84 | 1.23        | 1.33     |
| 11  | A16   | 155  | SER  | C-N   | 7.84  | 1.44        | 1.33     |
| 17  | F8    | 65   | ARG  | C-N   | -7.84 | 1.23        | 1.34     |
| 10  | C16   | 760  | GLY  | C-N   | -7.83 | 1.24        | 1.33     |
| 17  | F     | 65   | ARG  | C-N   | -7.83 | 1.23        | 1.34     |
| 10  | C8    | 471  | THR  | C-N   | -7.83 | 1.21        | 1.33     |
| 10  | C     | 471  | THR  | C-N   | -7.83 | 1.21        | 1.33     |
| 11  | A16   | 852  | ASP  | C-N   | -7.83 | 1.23        | 1.33     |
| 20  | E     | 349  | THR  | C-N   | 7.83  | 1.44        | 1.33     |
| 10  | C32   | 106  | GLY  | C-N   | -7.83 | 1.21        | 1.33     |
| 14  | W     | 658  | GLN  | C-N   | -7.82 | 1.23        | 1.33     |
| 11  | A40   | 852  | ASP  | C-N   | -7.82 | 1.23        | 1.33     |
| 18  | B     | 958  | ARG  | C-N   | 7.82  | 1.45        | 1.33     |
| 20  | E     | 462  | THR  | C-N   | -7.82 | 1.23        | 1.33     |
| 10  | C8    | 1277 | SER  | C-N   | -7.82 | 1.22        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A     | 852  | ASP  | C-N   | -7.82 | 1.23        | 1.33     |
| 18  | B8    | 492  | GLY  | C-N   | -7.82 | 1.23        | 1.33     |
| 9   | K8    | 1076 | ARG  | C-N   | -7.81 | 1.23        | 1.33     |
| 19  | 4     | 169  | CYS  | C-N   | -7.81 | 1.23        | 1.33     |
| 20  | E8    | 187  | GLY  | C-N   | -7.81 | 1.24        | 1.33     |
| 9   | K     | 787  | PRO  | C-N   | -7.81 | 1.23        | 1.33     |
| 13  | V     | 922  | TYR  | C-N   | -7.81 | 1.23        | 1.33     |
| 10  | C8    | 760  | GLY  | C-N   | -7.81 | 1.24        | 1.33     |
| 11  | A24   | 782  | PRO  | N-CD  | -7.81 | 1.36        | 1.47     |
| 15  | J     | 587  | ILE  | C-N   | -7.80 | 1.23        | 1.33     |
| 11  | A16   | 782  | PRO  | N-CD  | -7.80 | 1.36        | 1.47     |
| 10  | C32   | 1792 | GLU  | C-N   | -7.80 | 1.24        | 1.33     |
| 2   | M     | 783  | TRP  | C-N   | -7.80 | 1.22        | 1.33     |
| 18  | B     | 218  | LEU  | C-N   | -7.80 | 1.24        | 1.33     |
| 10  | C32   | 760  | GLY  | C-N   | -7.80 | 1.24        | 1.33     |
| 9   | K     | 613  | ALA  | C-N   | 7.80  | 1.43        | 1.33     |
| 20  | E     | 187  | GLY  | C-N   | -7.80 | 1.24        | 1.33     |
| 10  | C24   | 760  | GLY  | C-N   | -7.79 | 1.24        | 1.33     |
| 10  | C8    | 713  | ASP  | C-N   | -7.79 | 1.20        | 1.33     |
| 18  | B8    | 218  | LEU  | C-N   | -7.79 | 1.24        | 1.33     |
| 1   | R     | 1432 | LYS  | C-N   | -7.79 | 1.22        | 1.33     |
| 9   | K8    | 656  | LEU  | C-N   | -7.79 | 1.24        | 1.33     |
| 10  | C16   | 1792 | GLU  | C-N   | -7.79 | 1.24        | 1.33     |
| 11  | A40   | 782  | PRO  | N-CD  | -7.79 | 1.36        | 1.47     |
| 18  | B     | 589  | ASN  | C-N   | -7.79 | 1.23        | 1.34     |
| 11  | A24   | 852  | ASP  | C-N   | -7.79 | 1.23        | 1.33     |
| 10  | C24   | 1792 | GLU  | C-N   | -7.79 | 1.24        | 1.33     |
| 11  | A32   | 852  | ASP  | C-N   | -7.79 | 1.23        | 1.33     |
| 19  | 4     | 95   | THR  | C-N   | -7.79 | 1.23        | 1.33     |
| 9   | K8    | 613  | ALA  | C-N   | 7.79  | 1.43        | 1.33     |
| 19  | 4     | 155  | ASN  | C-N   | -7.78 | 1.22        | 1.33     |
| 14  | W     | 751  | LYS  | C-N   | 7.77  | 1.43        | 1.33     |
| 2   | M16   | 783  | TRP  | C-N   | -7.77 | 1.22        | 1.33     |
| 1   | R     | 1278 | LYS  | C-N   | -7.77 | 1.23        | 1.33     |
| 9   | K     | 1208 | GLN  | C-N   | -7.77 | 1.23        | 1.33     |
| 9   | K8    | 1208 | GLN  | C-N   | -7.77 | 1.23        | 1.33     |
| 1   | R16   | 1278 | LYS  | C-N   | -7.76 | 1.23        | 1.33     |
| 10  | C24   | 1251 | PHE  | C-N   | -7.76 | 1.24        | 1.33     |
| 11  | A32   | 782  | PRO  | N-CD  | -7.76 | 1.36        | 1.47     |
| 10  | C8    | 1792 | GLU  | C-N   | -7.75 | 1.24        | 1.33     |
| 9   | K8    | 787  | PRO  | C-N   | -7.75 | 1.23        | 1.33     |
| 5   | P16   | 449  | GLN  | C-N   | -7.75 | 1.23        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 492  | GLY  | C-N   | -7.75 | 1.24        | 1.33     |
| 10  | C32   | 713  | ASP  | C-N   | -7.75 | 1.20        | 1.33     |
| 1   | R8    | 1432 | LYS  | C-N   | -7.75 | 1.22        | 1.33     |
| 10  | C16   | 713  | ASP  | C-N   | -7.75 | 1.20        | 1.33     |
| 19  | 48    | 95   | THR  | C-N   | -7.74 | 1.23        | 1.33     |
| 11  | A24   | 26   | PRO  | N-CD  | -7.74 | 1.36        | 1.47     |
| 10  | C     | 713  | ASP  | C-N   | -7.74 | 1.20        | 1.33     |
| 23  | J8    | 630  | ASP  | C-N   | -7.74 | 1.22        | 1.33     |
| 11  | A32   | 411  | GLY  | C-N   | -7.74 | 1.22        | 1.33     |
| 2   | M8    | 832  | PRO  | C-N   | -7.73 | 1.23        | 1.33     |
| 1   | R8    | 1278 | LYS  | C-N   | -7.73 | 1.23        | 1.33     |
| 18  | B8    | 589  | ASN  | C-N   | -7.73 | 1.23        | 1.34     |
| 11  | A40   | 26   | PRO  | N-CD  | -7.73 | 1.36        | 1.47     |
| 10  | C8    | 663  | ILE  | C-N   | -7.73 | 1.23        | 1.33     |
| 12  | A48   | 782  | PRO  | N-CD  | -7.72 | 1.36        | 1.47     |
| 15  | J     | 591  | LYS  | C-N   | -7.72 | 1.24        | 1.33     |
| 18  | B     | 1921 | PRO  | C-N   | -7.72 | 1.25        | 1.33     |
| 23  | J32   | 630  | ASP  | C-N   | -7.72 | 1.23        | 1.33     |
| 12  | A     | 782  | PRO  | N-CD  | -7.72 | 1.36        | 1.47     |
| 10  | C     | 1251 | PHE  | C-N   | -7.71 | 1.24        | 1.33     |
| 10  | C24   | 663  | ILE  | C-N   | -7.71 | 1.23        | 1.33     |
| 2   | M8    | 783  | TRP  | C-N   | -7.71 | 1.22        | 1.33     |
| 13  | V     | 811  | MET  | C-N   | -7.71 | 1.23        | 1.33     |
| 18  | B     | 313  | ILE  | C-N   | 7.71  | 1.44        | 1.33     |
| 10  | C16   | 1251 | PHE  | C-N   | -7.71 | 1.24        | 1.33     |
| 13  | V     | 772  | GLY  | C-N   | -7.71 | 1.23        | 1.33     |
| 18  | B     | 507  | ASP  | C-N   | 7.71  | 1.43        | 1.33     |
| 2   | M     | 832  | PRO  | C-N   | -7.70 | 1.23        | 1.33     |
| 10  | C8    | 745  | SER  | C-N   | -7.70 | 1.25        | 1.33     |
| 19  | 48    | 155  | ASN  | C-N   | -7.70 | 1.22        | 1.33     |
| 12  | A48   | 852  | ASP  | C-N   | -7.70 | 1.23        | 1.33     |
| 6   | O8    | 177  | PRO  | N-CD  | -7.70 | 1.36        | 1.47     |
| 1   | R8    | 1215 | ASP  | C-N   | -7.70 | 1.24        | 1.34     |
| 10  | C     | 745  | SER  | C-N   | -7.69 | 1.25        | 1.33     |
| 18  | B     | 1135 | ASP  | C-N   | 7.69  | 1.44        | 1.33     |
| 18  | B8    | 1442 | GLY  | C-N   | 7.69  | 1.45        | 1.33     |
| 11  | A32   | 26   | PRO  | N-CD  | -7.68 | 1.36        | 1.47     |
| 11  | A16   | 26   | PRO  | N-CD  | -7.68 | 1.36        | 1.47     |
| 12  | A48   | 411  | GLY  | C-N   | -7.68 | 1.22        | 1.33     |
| 5   | P8    | 449  | GLN  | C-N   | -7.68 | 1.23        | 1.34     |
| 7   | Q16   | 325  | GLU  | C-N   | -7.67 | 1.23        | 1.33     |
| 18  | B8    | 1921 | PRO  | C-N   | -7.67 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 13  | V     | 810  | TYR  | C-N   | -7.67 | 1.23        | 1.33     |
| 11  | A40   | 411  | GLY  | C-N   | -7.67 | 1.22        | 1.33     |
| 18  | B8    | 1614 | GLU  | C-N   | -7.67 | 1.23        | 1.33     |
| 23  | J16   | 630  | ASP  | C-N   | -7.67 | 1.23        | 1.33     |
| 10  | C32   | 663  | ILE  | C-N   | -7.67 | 1.23        | 1.33     |
| 9   | K8    | 664  | GLU  | C-N   | -7.67 | 1.23        | 1.33     |
| 23  | J8    | 679  | GLU  | C-N   | 7.67  | 1.44        | 1.33     |
| 18  | B     | 536  | ILE  | C-N   | -7.66 | 1.22        | 1.33     |
| 10  | C     | 663  | ILE  | C-N   | -7.66 | 1.24        | 1.33     |
| 11  | A32   | 98   | ALA  | C-N   | -7.66 | 1.22        | 1.33     |
| 23  | J24   | 630  | ASP  | C-N   | -7.66 | 1.23        | 1.33     |
| 10  | C32   | 1251 | PHE  | C-N   | -7.66 | 1.24        | 1.33     |
| 18  | B     | 499  | ILE  | C-N   | 7.66  | 1.44        | 1.33     |
| 18  | B     | 1442 | GLY  | C-N   | 7.66  | 1.45        | 1.33     |
| 18  | B8    | 1195 | SER  | C-N   | -7.66 | 1.23        | 1.34     |
| 18  | B8    | 1135 | ASP  | C-N   | 7.65  | 1.44        | 1.33     |
| 10  | C16   | 663  | ILE  | C-N   | -7.65 | 1.24        | 1.33     |
| 18  | B8    | 536  | ILE  | C-N   | -7.65 | 1.22        | 1.33     |
| 18  | B     | 1614 | GLU  | C-N   | -7.65 | 1.23        | 1.33     |
| 18  | B8    | 476  | GLY  | C-N   | -7.65 | 1.24        | 1.33     |
| 10  | C24   | 1340 | PRO  | N-CD  | -7.64 | 1.37        | 1.47     |
| 10  | C32   | 916  | LEU  | C-N   | -7.64 | 1.22        | 1.33     |
| 11  | A24   | 411  | GLY  | C-N   | -7.64 | 1.22        | 1.33     |
| 10  | C24   | 916  | LEU  | C-N   | -7.64 | 1.22        | 1.33     |
| 21  | H     | 128  | ASP  | C-N   | -7.64 | 1.24        | 1.33     |
| 10  | C24   | 713  | ASP  | C-N   | -7.64 | 1.20        | 1.33     |
| 10  | C     | 916  | LEU  | C-N   | -7.63 | 1.22        | 1.33     |
| 18  | B8    | 313  | ILE  | C-N   | 7.63  | 1.44        | 1.33     |
| 10  | C8    | 1735 | TYR  | C-N   | -7.63 | 1.24        | 1.33     |
| 10  | C24   | 1805 | ASP  | C-N   | -7.63 | 1.23        | 1.33     |
| 21  | H16   | 202  | GLN  | C-N   | -7.63 | 1.23        | 1.33     |
| 6   | O     | 177  | PRO  | N-CD  | -7.63 | 1.37        | 1.47     |
| 7   | Q8    | 325  | GLU  | C-N   | -7.63 | 1.23        | 1.33     |
| 18  | B8    | 507  | ASP  | C-N   | 7.63  | 1.43        | 1.33     |
| 11  | A16   | 411  | GLY  | C-N   | -7.62 | 1.22        | 1.33     |
| 5   | P     | 449  | GLN  | C-N   | -7.62 | 1.23        | 1.34     |
| 10  | C8    | 1804 | ILE  | C-N   | 7.62  | 1.44        | 1.33     |
| 2   | M16   | 832  | PRO  | C-N   | -7.62 | 1.24        | 1.33     |
| 7   | Q     | 325  | GLU  | C-N   | -7.62 | 1.23        | 1.33     |
| 10  | C24   | 1735 | TYR  | C-N   | -7.62 | 1.24        | 1.33     |
| 10  | C24   | 1346 | PHE  | C-N   | -7.62 | 1.23        | 1.34     |
| 21  | H8    | 202  | GLN  | C-N   | -7.62 | 1.23        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C     | 1340 | PRO  | N-CD  | -7.62 | 1.37        | 1.47     |
| 10  | C16   | 1804 | ILE  | C-N   | 7.62  | 1.44        | 1.33     |
| 10  | C24   | 1707 | SER  | C-N   | -7.62 | 1.24        | 1.33     |
| 21  | H24   | 202  | GLN  | C-N   | -7.62 | 1.23        | 1.33     |
| 7   | Q8    | 95   | PHE  | C-N   | 7.62  | 1.44        | 1.34     |
| 10  | C8    | 1346 | PHE  | C-N   | -7.62 | 1.23        | 1.34     |
| 9   | K     | 664  | GLU  | C-N   | -7.61 | 1.24        | 1.33     |
| 10  | C16   | 592  | LEU  | C-N   | -7.61 | 1.23        | 1.33     |
| 10  | C16   | 1346 | PHE  | C-N   | -7.61 | 1.23        | 1.34     |
| 9   | K     | 1005 | LEU  | C-N   | -7.61 | 1.23        | 1.33     |
| 9   | K8    | 988  | PHE  | C-N   | -7.61 | 1.24        | 1.33     |
| 11  | A16   | 98   | ALA  | C-N   | -7.61 | 1.22        | 1.33     |
| 12  | A     | 411  | GLY  | C-N   | -7.61 | 1.22        | 1.33     |
| 10  | C8    | 1251 | PHE  | C-N   | -7.61 | 1.24        | 1.33     |
| 18  | B8    | 499  | ILE  | C-N   | 7.61  | 1.44        | 1.33     |
| 2   | M8    | 170  | ASP  | C-N   | -7.60 | 1.23        | 1.33     |
| 18  | B     | 429  | GLY  | C-N   | 7.60  | 1.43        | 1.33     |
| 18  | B8    | 429  | GLY  | C-N   | 7.60  | 1.43        | 1.33     |
| 23  | J32   | 679  | GLU  | C-N   | 7.60  | 1.44        | 1.33     |
| 10  | C16   | 1340 | PRO  | N-CD  | -7.60 | 1.37        | 1.47     |
| 10  | C32   | 1346 | PHE  | C-N   | -7.60 | 1.23        | 1.34     |
| 10  | C     | 1804 | ILE  | C-N   | 7.60  | 1.43        | 1.33     |
| 2   | M     | 738  | ILE  | C-N   | -7.59 | 1.23        | 1.33     |
| 10  | C16   | 916  | LEU  | C-N   | -7.59 | 1.23        | 1.33     |
| 6   | O16   | 177  | PRO  | N-CD  | -7.59 | 1.37        | 1.47     |
| 9   | K8    | 742  | GLU  | C-N   | -7.59 | 1.23        | 1.33     |
| 18  | B     | 393  | VAL  | C-N   | -7.59 | 1.24        | 1.33     |
| 21  | H     | 202  | GLN  | C-N   | -7.59 | 1.23        | 1.33     |
| 10  | C32   | 1340 | PRO  | N-CD  | -7.59 | 1.37        | 1.47     |
| 23  | J24   | 679  | GLU  | C-N   | 7.59  | 1.44        | 1.33     |
| 21  | H16   | 128  | ASP  | C-N   | -7.59 | 1.24        | 1.33     |
| 9   | K8    | 1005 | LEU  | C-N   | -7.59 | 1.23        | 1.33     |
| 2   | M     | 170  | ASP  | C-N   | -7.59 | 1.23        | 1.33     |
| 2   | M16   | 170  | ASP  | C-N   | -7.59 | 1.23        | 1.33     |
| 10  | C     | 1735 | TYR  | C-N   | -7.59 | 1.24        | 1.33     |
| 5   | P     | 114  | LYS  | C-N   | 7.58  | 1.44        | 1.33     |
| 2   | M     | 831  | LEU  | C-N   | -7.58 | 1.23        | 1.33     |
| 10  | C32   | 1805 | ASP  | C-N   | -7.58 | 1.23        | 1.33     |
| 18  | B8    | 1848 | VAL  | C-N   | 7.58  | 1.44        | 1.33     |
| 10  | C8    | 1340 | PRO  | N-CD  | -7.58 | 1.37        | 1.47     |
| 21  | H24   | 128  | ASP  | C-N   | -7.58 | 1.24        | 1.33     |
| 6   | O     | 102  | SER  | C-N   | -7.58 | 1.23        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 603  | PHE  | C-N   | 7.58  | 1.44        | 1.33     |
| 2   | M8    | 738  | ILE  | C-N   | -7.57 | 1.23        | 1.33     |
| 18  | B8    | 393  | VAL  | C-N   | -7.57 | 1.24        | 1.33     |
| 20  | E     | 438  | SER  | C-N   | -7.57 | 1.23        | 1.33     |
| 19  | 4     | 444  | HIS  | C-N   | -7.57 | 1.23        | 1.33     |
| 10  | C32   | 745  | SER  | C-N   | -7.57 | 1.25        | 1.33     |
| 7   | Q     | 170  | TYR  | C-N   | -7.57 | 1.23        | 1.33     |
| 10  | C     | 1346 | PHE  | C-N   | -7.57 | 1.23        | 1.34     |
| 18  | B     | 1848 | VAL  | C-N   | 7.57  | 1.44        | 1.33     |
| 23  | J16   | 679  | GLU  | C-N   | 7.57  | 1.44        | 1.33     |
| 7   | Q16   | 170  | TYR  | C-N   | -7.57 | 1.23        | 1.33     |
| 10  | C     | 1805 | ASP  | C-N   | -7.57 | 1.23        | 1.33     |
| 18  | B     | 1195 | SER  | C-N   | -7.57 | 1.23        | 1.34     |
| 10  | C24   | 745  | SER  | C-N   | -7.56 | 1.25        | 1.33     |
| 5   | P16   | 114  | LYS  | C-N   | 7.56  | 1.44        | 1.33     |
| 2   | M16   | 738  | ILE  | C-N   | -7.56 | 1.23        | 1.33     |
| 7   | Q8    | 170  | TYR  | C-N   | -7.56 | 1.23        | 1.33     |
| 10  | C24   | 725  | LEU  | C-N   | -7.56 | 1.24        | 1.33     |
| 10  | C8    | 1707 | SER  | C-N   | -7.56 | 1.24        | 1.33     |
| 10  | C32   | 1804 | ILE  | C-N   | 7.55  | 1.43        | 1.33     |
| 10  | C16   | 1707 | SER  | C-N   | -7.55 | 1.24        | 1.33     |
| 20  | E8    | 438  | SER  | C-N   | -7.55 | 1.23        | 1.33     |
| 15  | J     | 682  | ALA  | C-N   | 7.55  | 1.44        | 1.33     |
| 9   | K     | 757  | ALA  | C-N   | -7.55 | 1.23        | 1.33     |
| 9   | K8    | 581  | ASP  | C-N   | -7.55 | 1.23        | 1.34     |
| 10  | C16   | 1805 | ASP  | C-N   | -7.55 | 1.23        | 1.33     |
| 15  | J     | 588  | GLU  | C-N   | -7.55 | 1.24        | 1.33     |
| 10  | C     | 559  | ASN  | C-N   | 7.55  | 1.43        | 1.33     |
| 18  | B     | 1484 | ALA  | C-N   | 7.55  | 1.44        | 1.33     |
| 21  | H16   | 153  | SER  | C-N   | -7.55 | 1.25        | 1.33     |
| 10  | C32   | 1735 | TYR  | C-N   | -7.54 | 1.24        | 1.33     |
| 10  | C8    | 559  | ASN  | C-N   | 7.54  | 1.43        | 1.33     |
| 9   | K     | 988  | PHE  | C-N   | -7.54 | 1.24        | 1.33     |
| 5   | P8    | 114  | LYS  | C-N   | 7.54  | 1.44        | 1.33     |
| 10  | C24   | 559  | ASN  | C-N   | 7.54  | 1.43        | 1.33     |
| 19  | 48    | 444  | HIS  | C-N   | -7.54 | 1.23        | 1.33     |
| 2   | M8    | 383  | SER  | C-N   | -7.54 | 1.23        | 1.33     |
| 10  | C     | 1707 | SER  | C-N   | -7.54 | 1.24        | 1.33     |
| 21  | H8    | 128  | ASP  | C-N   | -7.54 | 1.24        | 1.33     |
| 9   | K     | 581  | ASP  | C-N   | -7.53 | 1.23        | 1.34     |
| 10  | C16   | 745  | SER  | C-N   | -7.53 | 1.25        | 1.33     |
| 22  | I16   | 369  | HIS  | C-N   | 7.53  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 14  | W     | 794  | LYS  | C-N   | -7.53 | 1.24        | 1.33     |
| 9   | K     | 1147 | LYS  | C-N   | -7.53 | 1.24        | 1.33     |
| 10  | C16   | 559  | ASN  | C-N   | 7.53  | 1.43        | 1.33     |
| 10  | C8    | 916  | LEU  | C-N   | -7.53 | 1.23        | 1.33     |
| 7   | Q     | 145  | GLY  | C-N   | -7.53 | 1.23        | 1.33     |
| 13  | V     | 918  | LYS  | C-N   | -7.53 | 1.23        | 1.33     |
| 2   | M16   | 383  | SER  | C-N   | -7.52 | 1.23        | 1.33     |
| 10  | C     | 592  | LEU  | C-N   | -7.52 | 1.23        | 1.33     |
| 2   | M8    | 831  | LEU  | C-N   | -7.52 | 1.23        | 1.33     |
| 9   | K8    | 757  | ALA  | C-N   | -7.52 | 1.23        | 1.33     |
| 10  | C8    | 592  | LEU  | C-N   | -7.52 | 1.23        | 1.33     |
| 6   | O8    | 102  | SER  | C-N   | -7.52 | 1.24        | 1.33     |
| 18  | B8    | 1001 | THR  | C-N   | -7.52 | 1.24        | 1.33     |
| 18  | B     | 476  | GLY  | C-N   | -7.52 | 1.24        | 1.33     |
| 18  | B     | 603  | PHE  | C-N   | 7.52  | 1.43        | 1.33     |
| 22  | I24   | 369  | HIS  | C-N   | 7.51  | 1.44        | 1.33     |
| 10  | C16   | 1502 | ARG  | C-N   | -7.51 | 1.23        | 1.33     |
| 10  | C32   | 592  | LEU  | C-N   | -7.51 | 1.23        | 1.33     |
| 18  | B8    | 1552 | LYS  | C-N   | 7.50  | 1.44        | 1.33     |
| 2   | M16   | 763  | ASP  | C-N   | -7.50 | 1.23        | 1.33     |
| 10  | C     | 725  | LEU  | C-N   | -7.50 | 1.24        | 1.33     |
| 9   | K     | 1040 | THR  | C-N   | -7.50 | 1.24        | 1.33     |
| 9   | K     | 742  | GLU  | C-N   | -7.50 | 1.23        | 1.33     |
| 6   | O16   | 102  | SER  | C-N   | -7.49 | 1.24        | 1.33     |
| 10  | C8    | 1805 | ASP  | C-N   | -7.49 | 1.23        | 1.33     |
| 9   | K8    | 1110 | GLN  | C-N   | -7.49 | 1.24        | 1.34     |
| 22  | I8    | 369  | HIS  | C-N   | 7.49  | 1.44        | 1.33     |
| 2   | M16   | 324  | GLU  | C-N   | 7.49  | 1.44        | 1.33     |
| 10  | C     | 356  | PHE  | C-N   | 7.49  | 1.44        | 1.34     |
| 2   | M8    | 763  | ASP  | C-N   | -7.49 | 1.23        | 1.33     |
| 9   | K8    | 1147 | LYS  | C-N   | -7.49 | 1.24        | 1.33     |
| 10  | C16   | 1735 | TYR  | C-N   | -7.49 | 1.24        | 1.33     |
| 10  | C8    | 356  | PHE  | C-N   | 7.48  | 1.44        | 1.34     |
| 10  | C16   | 725  | LEU  | C-N   | -7.48 | 1.24        | 1.33     |
| 18  | B     | 1530 | THR  | C-N   | 7.48  | 1.45        | 1.33     |
| 9   | K8    | 1043 | THR  | C-N   | -7.48 | 1.24        | 1.34     |
| 18  | B8    | 1530 | THR  | C-N   | 7.48  | 1.45        | 1.33     |
| 23  | J32   | 685  | GLY  | C-N   | -7.48 | 1.23        | 1.33     |
| 10  | C32   | 435  | SER  | C-N   | 7.48  | 1.44        | 1.33     |
| 2   | M     | 634  | ARG  | C-N   | -7.48 | 1.24        | 1.33     |
| 18  | B     | 1552 | LYS  | C-N   | 7.48  | 1.44        | 1.33     |
| 6   | O8    | 325  | PRO  | N-CD  | -7.47 | 1.37        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 6   | O16   | 325  | PRO  | N-CD  | -7.47 | 1.37        | 1.47     |
| 19  | 48    | 275  | ASP  | C-N   | -7.47 | 1.22        | 1.33     |
| 22  | I     | 369  | HIS  | C-N   | 7.47  | 1.44        | 1.33     |
| 2   | M     | 324  | GLU  | C-N   | 7.47  | 1.44        | 1.33     |
| 2   | M     | 763  | ASP  | C-N   | -7.47 | 1.23        | 1.33     |
| 9   | K8    | 1223 | ASP  | C-N   | 7.47  | 1.44        | 1.33     |
| 18  | B8    | 1484 | ALA  | C-N   | 7.47  | 1.44        | 1.33     |
| 20  | E8    | 454  | MET  | C-N   | -7.47 | 1.24        | 1.33     |
| 10  | C32   | 559  | ASN  | C-N   | 7.47  | 1.43        | 1.33     |
| 18  | B8    | 588  | PHE  | C-N   | 7.47  | 1.43        | 1.33     |
| 19  | 4     | 275  | ASP  | C-N   | -7.47 | 1.22        | 1.33     |
| 1   | R16   | 1238 | GLY  | C-N   | 7.47  | 1.43        | 1.33     |
| 20  | E     | 252  | LYS  | C-N   | -7.47 | 1.22        | 1.33     |
| 10  | C32   | 725  | LEU  | C-N   | -7.47 | 1.24        | 1.33     |
| 10  | C32   | 1707 | SER  | C-N   | -7.47 | 1.24        | 1.33     |
| 2   | M8    | 324  | GLU  | C-N   | 7.46  | 1.44        | 1.33     |
| 7   | Q8    | 145  | GLY  | C-N   | -7.46 | 1.23        | 1.33     |
| 20  | E     | 454  | MET  | C-N   | -7.46 | 1.24        | 1.33     |
| 1   | R     | 1173 | PRO  | N-CD  | -7.46 | 1.37        | 1.47     |
| 2   | M     | 383  | SER  | C-N   | -7.46 | 1.23        | 1.33     |
| 6   | O     | 325  | PRO  | N-CD  | -7.46 | 1.37        | 1.47     |
| 10  | C32   | 1502 | ARG  | C-N   | -7.46 | 1.23        | 1.33     |
| 1   | R16   | 1173 | PRO  | N-CD  | -7.45 | 1.37        | 1.47     |
| 2   | M16   | 831  | LEU  | C-N   | -7.45 | 1.23        | 1.33     |
| 2   | M8    | 634  | ARG  | C-N   | -7.45 | 1.24        | 1.33     |
| 10  | C8    | 435  | SER  | C-N   | 7.45  | 1.44        | 1.33     |
| 9   | K8    | 1040 | THR  | C-N   | -7.45 | 1.24        | 1.33     |
| 10  | C24   | 1804 | ILE  | C-N   | 7.45  | 1.43        | 1.33     |
| 10  | C     | 1502 | ARG  | C-N   | -7.45 | 1.23        | 1.33     |
| 10  | C8    | 808  | PRO  | N-CD  | -7.45 | 1.37        | 1.47     |
| 21  | H24   | 153  | SER  | C-N   | -7.45 | 1.25        | 1.33     |
| 9   | K     | 1110 | GLN  | C-N   | -7.44 | 1.24        | 1.34     |
| 1   | R8    | 1173 | PRO  | N-CD  | -7.44 | 1.37        | 1.47     |
| 7   | Q16   | 145  | GLY  | C-N   | -7.44 | 1.23        | 1.33     |
| 20  | E8    | 252  | LYS  | C-N   | -7.44 | 1.22        | 1.33     |
| 18  | B8    | 1943 | HIS  | C-N   | -7.44 | 1.24        | 1.34     |
| 10  | C     | 808  | PRO  | N-CD  | -7.44 | 1.37        | 1.47     |
| 18  | B     | 1001 | THR  | C-N   | -7.44 | 1.24        | 1.33     |
| 22  | I24   | 256  | LYS  | C-N   | 7.44  | 1.43        | 1.33     |
| 9   | K     | 1023 | LEU  | C-N   | -7.43 | 1.24        | 1.33     |
| 10  | C16   | 435  | SER  | C-N   | 7.43  | 1.44        | 1.33     |
| 21  | H     | 153  | SER  | C-N   | -7.43 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 356  | PHE  | C-N   | 7.43  | 1.44        | 1.34     |
| 20  | E8    | 92   | PRO  | C-N   | -7.43 | 1.23        | 1.33     |
| 9   | K8    | 723  | ALA  | C-N   | 7.42  | 1.44        | 1.33     |
| 14  | W     | 604  | PRO  | C-N   | 7.42  | 1.44        | 1.34     |
| 1   | R8    | 1212 | SER  | C-N   | -7.42 | 1.23        | 1.33     |
| 10  | C8    | 1502 | ARG  | C-N   | -7.42 | 1.23        | 1.33     |
| 2   | M16   | 634  | ARG  | C-N   | -7.42 | 1.24        | 1.33     |
| 10  | C16   | 808  | PRO  | N-CD  | -7.42 | 1.37        | 1.47     |
| 10  | C24   | 592  | LEU  | C-N   | -7.42 | 1.23        | 1.33     |
| 23  | J8    | 685  | GLY  | C-N   | -7.42 | 1.23        | 1.33     |
| 23  | J24   | 685  | GLY  | C-N   | -7.42 | 1.23        | 1.33     |
| 18  | B8    | 820  | ARG  | C-N   | 7.41  | 1.44        | 1.33     |
| 10  | C8    | 1776 | SER  | C-N   | 7.41  | 1.45        | 1.33     |
| 18  | B8    | 1543 | HIS  | C-N   | -7.41 | 1.24        | 1.33     |
| 22  | I16   | 256  | LYS  | C-N   | 7.41  | 1.43        | 1.33     |
| 18  | B8    | 618  | VAL  | C-N   | -7.41 | 1.24        | 1.34     |
| 20  | E     | 493  | TRP  | C-N   | -7.41 | 1.25        | 1.33     |
| 10  | C24   | 1502 | ARG  | C-N   | -7.41 | 1.23        | 1.33     |
| 13  | V     | 745  | LEU  | C-N   | -7.41 | 1.24        | 1.33     |
| 18  | B     | 1543 | HIS  | C-N   | -7.41 | 1.24        | 1.33     |
| 23  | J16   | 685  | GLY  | C-N   | -7.41 | 1.23        | 1.33     |
| 10  | C32   | 535  | MET  | C-N   | -7.40 | 1.24        | 1.33     |
| 1   | R     | 1238 | GLY  | C-N   | 7.40  | 1.43        | 1.33     |
| 5   | P8    | 379  | GLY  | C-N   | -7.40 | 1.23        | 1.33     |
| 10  | C     | 1776 | SER  | C-N   | 7.40  | 1.44        | 1.33     |
| 11  | A16   | 858  | ALA  | C-N   | -7.40 | 1.23        | 1.34     |
| 1   | R     | 1212 | SER  | C-N   | -7.40 | 1.23        | 1.33     |
| 3   | N     | 168  | VAL  | C-N   | -7.40 | 1.23        | 1.33     |
| 9   | K     | 680  | CYS  | C-N   | -7.40 | 1.23        | 1.33     |
| 10  | C16   | 395  | CYS  | C-N   | -7.40 | 1.23        | 1.33     |
| 10  | C24   | 356  | PHE  | C-N   | 7.40  | 1.44        | 1.34     |
| 3   | N8    | 168  | VAL  | C-N   | -7.39 | 1.23        | 1.33     |
| 10  | C     | 395  | CYS  | C-N   | -7.39 | 1.23        | 1.33     |
| 20  | E8    | 493  | TRP  | C-N   | -7.39 | 1.25        | 1.33     |
| 11  | A32   | 858  | ALA  | C-N   | -7.39 | 1.23        | 1.34     |
| 22  | I8    | 256  | LYS  | C-N   | 7.39  | 1.43        | 1.33     |
| 18  | B     | 1943 | HIS  | C-N   | -7.39 | 1.24        | 1.34     |
| 20  | E     | 428  | GLY  | C-N   | 7.39  | 1.51        | 1.33     |
| 10  | C16   | 687  | LYS  | C-N   | -7.39 | 1.23        | 1.34     |
| 9   | K8    | 680  | CYS  | C-N   | -7.39 | 1.23        | 1.33     |
| 10  | C32   | 356  | PHE  | C-N   | 7.38  | 1.44        | 1.34     |
| 10  | C32   | 808  | PRO  | N-CD  | -7.38 | 1.37        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 1776 | SER  | C-N   | 7.38  | 1.44        | 1.33     |
| 1   | R8    | 1238 | GLY  | C-N   | 7.38  | 1.43        | 1.33     |
| 9   | K8    | 1180 | TRP  | C-N   | 7.38  | 1.44        | 1.34     |
| 10  | C24   | 1350 | ASN  | C-N   | -7.38 | 1.24        | 1.33     |
| 5   | P16   | 379  | GLY  | C-N   | -7.38 | 1.23        | 1.33     |
| 10  | C8    | 687  | LYS  | C-N   | -7.38 | 1.23        | 1.34     |
| 21  | H16   | 291  | VAL  | C-N   | 7.38  | 1.43        | 1.33     |
| 9   | K     | 727  | ASP  | C-N   | -7.38 | 1.23        | 1.33     |
| 10  | C24   | 1776 | SER  | C-N   | 7.38  | 1.44        | 1.33     |
| 20  | E8    | 428  | GLY  | C-N   | 7.38  | 1.51        | 1.33     |
| 12  | A48   | 858  | ALA  | C-N   | -7.38 | 1.23        | 1.34     |
| 18  | B     | 618  | VAL  | C-N   | -7.38 | 1.24        | 1.34     |
| 1   | R16   | 1426 | ALA  | C-N   | -7.37 | 1.22        | 1.33     |
| 10  | C16   | 1350 | ASN  | C-N   | -7.37 | 1.24        | 1.33     |
| 22  | I24   | 368  | VAL  | C-N   | 7.37  | 1.48        | 1.33     |
| 10  | C16   | 535  | MET  | C-N   | -7.37 | 1.24        | 1.33     |
| 21  | H8    | 153  | SER  | C-N   | -7.37 | 1.25        | 1.33     |
| 10  | C24   | 808  | PRO  | N-CD  | -7.37 | 1.37        | 1.47     |
| 22  | I     | 368  | VAL  | C-N   | 7.37  | 1.48        | 1.33     |
| 5   | P     | 243  | VAL  | C-N   | -7.37 | 1.23        | 1.33     |
| 9   | K8    | 1023 | LEU  | C-N   | -7.37 | 1.24        | 1.33     |
| 22  | I     | 256  | LYS  | C-N   | 7.37  | 1.43        | 1.33     |
| 2   | M     | 793  | VAL  | C-N   | -7.37 | 1.24        | 1.33     |
| 9   | K     | 1223 | ASP  | C-N   | 7.37  | 1.44        | 1.33     |
| 13  | V     | 768  | GLU  | C-N   | -7.37 | 1.24        | 1.33     |
| 20  | E     | 92   | PRO  | C-N   | -7.36 | 1.24        | 1.33     |
| 10  | C     | 1739 | VAL  | C-N   | -7.36 | 1.24        | 1.33     |
| 22  | I16   | 368  | VAL  | C-N   | 7.36  | 1.48        | 1.33     |
| 2   | M16   | 665  | HIS  | C-N   | -7.36 | 1.24        | 1.33     |
| 9   | K     | 1043 | THR  | C-N   | -7.36 | 1.24        | 1.34     |
| 10  | C24   | 535  | MET  | C-N   | -7.36 | 1.24        | 1.33     |
| 21  | H8    | 291  | VAL  | C-N   | 7.36  | 1.43        | 1.33     |
| 10  | C32   | 1776 | SER  | C-N   | 7.36  | 1.44        | 1.33     |
| 11  | A40   | 858  | ALA  | C-N   | -7.36 | 1.23        | 1.34     |
| 10  | C     | 435  | SER  | C-N   | 7.36  | 1.43        | 1.33     |
| 23  | J16   | 631  | GLU  | C-N   | -7.36 | 1.24        | 1.33     |
| 3   | N16   | 168  | VAL  | C-N   | -7.35 | 1.23        | 1.33     |
| 12  | A     | 858  | ALA  | C-N   | -7.35 | 1.23        | 1.34     |
| 10  | C8    | 1739 | VAL  | C-N   | -7.35 | 1.24        | 1.33     |
| 1   | R     | 1215 | ASP  | C-N   | -7.35 | 1.24        | 1.33     |
| 1   | R8    | 1426 | ALA  | C-N   | -7.35 | 1.23        | 1.33     |
| 10  | C24   | 1505 | MET  | C-N   | 7.35  | 1.43        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 687  | LYS  | C-N   | -7.35 | 1.23        | 1.34     |
| 10  | C     | 1505 | MET  | C-N   | 7.35  | 1.43        | 1.34     |
| 22  | I16   | 102  | PRO  | N-CD  | -7.35 | 1.37        | 1.47     |
| 9   | K     | 723  | ALA  | C-N   | 7.35  | 1.44        | 1.33     |
| 22  | I     | 102  | PRO  | N-CD  | -7.35 | 1.37        | 1.47     |
| 1   | R16   | 1215 | ASP  | C-N   | -7.34 | 1.24        | 1.33     |
| 5   | P     | 379  | GLY  | C-N   | -7.34 | 1.24        | 1.33     |
| 18  | B     | 1227 | TYR  | C-N   | 7.34  | 1.44        | 1.33     |
| 22  | I8    | 368  | VAL  | C-N   | 7.34  | 1.48        | 1.33     |
| 18  | B     | 1408 | ALA  | C-N   | -7.34 | 1.24        | 1.33     |
| 10  | C32   | 1350 | ASN  | C-N   | -7.34 | 1.24        | 1.33     |
| 10  | C     | 687  | LYS  | C-N   | -7.34 | 1.23        | 1.34     |
| 19  | 4     | 374  | GLY  | C-N   | -7.34 | 1.24        | 1.33     |
| 10  | C24   | 435  | SER  | C-N   | 7.34  | 1.43        | 1.33     |
| 10  | C32   | 1505 | MET  | C-N   | 7.34  | 1.43        | 1.34     |
| 19  | 48    | 233  | ASP  | C-N   | -7.34 | 1.22        | 1.33     |
| 23  | J8    | 631  | GLU  | C-N   | -7.34 | 1.24        | 1.33     |
| 11  | A24   | 858  | ALA  | C-N   | -7.33 | 1.23        | 1.34     |
| 20  | E8    | 442  | LYS  | C-N   | -7.33 | 1.23        | 1.33     |
| 10  | C8    | 395  | CYS  | C-N   | -7.33 | 1.24        | 1.33     |
| 10  | C8    | 1350 | ASN  | C-N   | -7.33 | 1.24        | 1.33     |
| 18  | B     | 1008 | ARG  | C-N   | -7.33 | 1.24        | 1.33     |
| 3   | N16   | 163  | ALA  | C-N   | -7.33 | 1.16        | 1.33     |
| 2   | M8    | 793  | VAL  | C-N   | -7.33 | 1.24        | 1.33     |
| 1   | R16   | 1212 | SER  | C-N   | -7.33 | 1.23        | 1.33     |
| 5   | P8    | 243  | VAL  | C-N   | -7.33 | 1.23        | 1.33     |
| 10  | C24   | 395  | CYS  | C-N   | -7.33 | 1.24        | 1.33     |
| 18  | B8    | 1008 | ARG  | C-N   | -7.33 | 1.24        | 1.33     |
| 22  | I24   | 102  | PRO  | N-CD  | -7.33 | 1.37        | 1.47     |
| 1   | R     | 1426 | ALA  | C-N   | -7.32 | 1.23        | 1.33     |
| 3   | N     | 246  | GLU  | C-N   | -7.32 | 1.21        | 1.33     |
| 3   | N8    | 163  | ALA  | C-N   | -7.32 | 1.16        | 1.33     |
| 9   | K     | 1180 | TRP  | C-N   | 7.32  | 1.44        | 1.34     |
| 5   | P16   | 243  | VAL  | C-N   | -7.32 | 1.23        | 1.33     |
| 19  | 48    | 142  | ASP  | C-N   | -7.32 | 1.23        | 1.33     |
| 21  | H24   | 291  | VAL  | C-N   | 7.32  | 1.43        | 1.33     |
| 10  | C32   | 1666 | LYS  | C-N   | 7.32  | 1.44        | 1.33     |
| 10  | C8    | 1505 | MET  | C-N   | 7.31  | 1.43        | 1.34     |
| 2   | M8    | 455  | GLU  | C-N   | -7.30 | 1.24        | 1.33     |
| 2   | M8    | 665  | HIS  | C-N   | -7.30 | 1.24        | 1.33     |
| 21  | H     | 291  | VAL  | C-N   | 7.30  | 1.43        | 1.33     |
| 3   | N     | 163  | ALA  | C-N   | -7.30 | 1.16        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K8    | 849  | LEU  | C-N   | -7.30 | 1.23        | 1.34     |
| 18  | B     | 1061 | ALA  | C-N   | 7.30  | 1.44        | 1.33     |
| 10  | C16   | 1666 | LYS  | C-N   | 7.30  | 1.44        | 1.33     |
| 10  | C24   | 1141 | ASP  | C-N   | -7.30 | 1.23        | 1.33     |
| 2   | M16   | 455  | GLU  | C-N   | -7.30 | 1.24        | 1.33     |
| 10  | C     | 1141 | ASP  | C-N   | -7.30 | 1.23        | 1.33     |
| 10  | C     | 1350 | ASN  | C-N   | -7.30 | 1.24        | 1.33     |
| 18  | B8    | 35   | PRO  | N-CD  | -7.30 | 1.37        | 1.47     |
| 1   | R16   | 1464 | CYS  | C-N   | 7.29  | 1.44        | 1.34     |
| 18  | B8    | 1227 | TYR  | C-N   | 7.29  | 1.44        | 1.33     |
| 1   | R     | 1464 | CYS  | C-N   | 7.29  | 1.44        | 1.34     |
| 9   | K     | 818  | MET  | C-N   | -7.29 | 1.23        | 1.33     |
| 18  | B     | 35   | PRO  | N-CD  | -7.29 | 1.37        | 1.47     |
| 18  | B8    | 1061 | ALA  | C-N   | 7.29  | 1.44        | 1.33     |
| 3   | N8    | 46   | SER  | C-N   | 7.29  | 1.43        | 1.33     |
| 5   | P     | 289  | PRO  | N-CD  | -7.29 | 1.37        | 1.47     |
| 10  | C24   | 1666 | LYS  | C-N   | 7.29  | 1.43        | 1.33     |
| 22  | I8    | 102  | PRO  | N-CD  | -7.29 | 1.37        | 1.47     |
| 10  | C32   | 344  | ASP  | C-N   | -7.29 | 1.24        | 1.33     |
| 3   | N     | 46   | SER  | C-N   | 7.28  | 1.43        | 1.33     |
| 10  | C     | 1666 | LYS  | C-N   | 7.28  | 1.43        | 1.33     |
| 1   | R8    | 1464 | CYS  | C-N   | 7.28  | 1.44        | 1.34     |
| 10  | C16   | 1505 | MET  | C-N   | 7.28  | 1.43        | 1.34     |
| 18  | B     | 820  | ARG  | C-N   | 7.28  | 1.44        | 1.33     |
| 2   | M     | 665  | HIS  | C-N   | -7.28 | 1.24        | 1.33     |
| 9   | K8    | 1162 | ASN  | C-N   | -7.28 | 1.23        | 1.33     |
| 18  | B     | 1803 | THR  | C-N   | 7.28  | 1.43        | 1.33     |
| 10  | C32   | 395  | CYS  | C-N   | -7.28 | 1.24        | 1.33     |
| 10  | C32   | 687  | LYS  | C-N   | -7.28 | 1.24        | 1.34     |
| 19  | 4     | 233  | ASP  | C-N   | -7.28 | 1.23        | 1.33     |
| 19  | 48    | 374  | GLY  | C-N   | -7.28 | 1.24        | 1.33     |
| 3   | N8    | 246  | GLU  | C-N   | -7.27 | 1.21        | 1.33     |
| 9   | K     | 1047 | SER  | C-N   | 7.27  | 1.43        | 1.33     |
| 9   | K     | 1162 | ASN  | C-N   | -7.27 | 1.23        | 1.33     |
| 10  | C8    | 1141 | ASP  | C-N   | -7.27 | 1.23        | 1.33     |
| 20  | E     | 442  | LYS  | C-N   | -7.27 | 1.23        | 1.33     |
| 23  | J24   | 631  | GLU  | C-N   | -7.27 | 1.24        | 1.33     |
| 19  | 4     | 142  | ASP  | C-N   | -7.27 | 1.23        | 1.33     |
| 3   | N16   | 246  | GLU  | C-N   | -7.26 | 1.21        | 1.33     |
| 9   | K     | 849  | LEU  | C-N   | -7.26 | 1.24        | 1.34     |
| 18  | B8    | 1803 | THR  | C-N   | 7.26  | 1.43        | 1.33     |
| 10  | C32   | 1141 | ASP  | C-N   | -7.26 | 1.23        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M     | 455  | GLU  | C-N   | -7.25 | 1.24        | 1.33     |
| 2   | M16   | 793  | VAL  | C-N   | -7.25 | 1.24        | 1.33     |
| 9   | K8    | 727  | ASP  | C-N   | -7.25 | 1.23        | 1.33     |
| 9   | K     | 777  | GLN  | C-N   | -7.25 | 1.24        | 1.34     |
| 10  | C16   | 1739 | VAL  | C-N   | -7.25 | 1.24        | 1.33     |
| 7   | Q16   | 322  | GLU  | C-N   | -7.25 | 1.24        | 1.33     |
| 10  | C32   | 1739 | VAL  | C-N   | -7.25 | 1.24        | 1.33     |
| 12  | A48   | 605  | SER  | C-N   | -7.25 | 1.23        | 1.33     |
| 9   | K8    | 777  | GLN  | C-N   | -7.25 | 1.24        | 1.34     |
| 9   | K8    | 818  | MET  | C-N   | -7.24 | 1.23        | 1.33     |
| 23  | J32   | 631  | GLU  | C-N   | -7.24 | 1.24        | 1.33     |
| 9   | K8    | 1047 | SER  | C-N   | 7.24  | 1.43        | 1.33     |
| 3   | N16   | 46   | SER  | C-N   | 7.24  | 1.43        | 1.33     |
| 7   | Q     | 254  | ALA  | C-N   | -7.24 | 1.24        | 1.33     |
| 9   | K     | 762  | SER  | C-N   | -7.24 | 1.24        | 1.33     |
| 10  | C16   | 1141 | ASP  | C-N   | -7.24 | 1.23        | 1.33     |
| 11  | A24   | 321  | ILE  | C-N   | -7.24 | 1.23        | 1.33     |
| 7   | Q     | 227  | SER  | C-N   | -7.24 | 1.24        | 1.33     |
| 5   | P16   | 532  | SER  | C-N   | -7.24 | 1.24        | 1.33     |
| 10  | C     | 344  | ASP  | C-N   | -7.24 | 1.24        | 1.33     |
| 21  | H     | 329  | LYS  | C-N   | -7.23 | 1.24        | 1.33     |
| 10  | C24   | 714  | GLY  | C-N   | 7.23  | 1.43        | 1.33     |
| 10  | C32   | 715  | PHE  | C-N   | 7.23  | 1.43        | 1.33     |
| 9   | K8    | 731  | CYS  | C-N   | 7.23  | 1.43        | 1.33     |
| 10  | C24   | 344  | ASP  | C-N   | -7.23 | 1.24        | 1.33     |
| 18  | B8    | 1408 | ALA  | C-N   | -7.23 | 1.24        | 1.33     |
| 18  | B     | 1780 | LEU  | C-N   | -7.23 | 1.24        | 1.33     |
| 18  | B     | 976  | SER  | C-N   | 7.23  | 1.42        | 1.33     |
| 11  | A40   | 605  | SER  | C-N   | -7.22 | 1.23        | 1.33     |
| 10  | C8    | 535  | MET  | C-N   | -7.22 | 1.24        | 1.33     |
| 21  | H24   | 164  | ALA  | C-N   | -7.22 | 1.22        | 1.33     |
| 9   | K     | 731  | CYS  | C-N   | 7.22  | 1.43        | 1.33     |
| 12  | A     | 605  | SER  | C-N   | -7.22 | 1.23        | 1.33     |
| 10  | C     | 535  | MET  | C-N   | -7.22 | 1.24        | 1.33     |
| 18  | B8    | 976  | SER  | C-N   | 7.22  | 1.42        | 1.33     |
| 5   | P16   | 289  | PRO  | N-CD  | -7.22 | 1.37        | 1.47     |
| 6   | O16   | 149  | LEU  | C-N   | -7.22 | 1.23        | 1.33     |
| 18  | B8    | 243  | GLY  | C-N   | -7.22 | 1.24        | 1.33     |
| 21  | H24   | 329  | LYS  | C-N   | -7.22 | 1.24        | 1.33     |
| 10  | C     | 1348 | LEU  | C-N   | 7.22  | 1.43        | 1.34     |
| 10  | C32   | 1348 | LEU  | C-N   | 7.21  | 1.43        | 1.34     |
| 7   | Q     | 322  | GLU  | C-N   | -7.21 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 627  | VAL  | C-N   | 7.21  | 1.44        | 1.33     |
| 7   | Q8    | 322  | GLU  | C-N   | -7.21 | 1.24        | 1.33     |
| 10  | C16   | 715  | PHE  | C-N   | 7.21  | 1.43        | 1.33     |
| 5   | P16   | 599  | ASP  | C-N   | -7.21 | 1.24        | 1.33     |
| 9   | K     | 1106 | LEU  | C-N   | -7.20 | 1.24        | 1.33     |
| 10  | C24   | 1591 | LYS  | C-N   | 7.20  | 1.41        | 1.33     |
| 5   | P8    | 289  | PRO  | N-CD  | -7.20 | 1.37        | 1.47     |
| 10  | C     | 606  | MET  | C-N   | -7.20 | 1.24        | 1.33     |
| 5   | P8    | 599  | ASP  | C-N   | -7.20 | 1.24        | 1.33     |
| 9   | K8    | 812  | TYR  | C-N   | -7.20 | 1.24        | 1.33     |
| 9   | K8    | 957  | ILE  | C-N   | -7.20 | 1.24        | 1.33     |
| 9   | K     | 810  | LEU  | C-N   | -7.20 | 1.24        | 1.33     |
| 21  | H16   | 329  | LYS  | C-N   | -7.20 | 1.24        | 1.33     |
| 6   | O     | 149  | LEU  | C-N   | -7.20 | 1.24        | 1.33     |
| 10  | C32   | 606  | MET  | C-N   | -7.20 | 1.24        | 1.33     |
| 7   | Q8    | 254  | ALA  | C-N   | -7.19 | 1.24        | 1.33     |
| 5   | P8    | 532  | SER  | C-N   | -7.19 | 1.24        | 1.33     |
| 6   | O8    | 203  | ILE  | C-N   | -7.19 | 1.24        | 1.33     |
| 10  | C16   | 1348 | LEU  | C-N   | 7.19  | 1.43        | 1.34     |
| 11  | A24   | 605  | SER  | C-N   | -7.19 | 1.23        | 1.33     |
| 21  | H16   | 164  | ALA  | C-N   | -7.19 | 1.22        | 1.33     |
| 2   | M16   | 465  | GLY  | C-N   | 7.19  | 1.43        | 1.33     |
| 10  | C24   | 606  | MET  | C-N   | -7.19 | 1.24        | 1.33     |
| 18  | B     | 243  | GLY  | C-N   | -7.19 | 1.24        | 1.33     |
| 11  | A32   | 605  | SER  | C-N   | -7.18 | 1.23        | 1.33     |
| 21  | H     | 156  | GLU  | C-N   | -7.18 | 1.24        | 1.33     |
| 5   | P     | 532  | SER  | C-N   | -7.18 | 1.24        | 1.33     |
| 10  | C     | 1591 | LYS  | C-N   | 7.18  | 1.41        | 1.33     |
| 11  | A16   | 605  | SER  | C-N   | -7.18 | 1.23        | 1.33     |
| 2   | M     | 465  | GLY  | C-N   | 7.18  | 1.43        | 1.33     |
| 9   | K     | 812  | TYR  | C-N   | -7.18 | 1.24        | 1.33     |
| 9   | K     | 1245 | GLU  | C-N   | -7.18 | 1.24        | 1.34     |
| 10  | C24   | 650  | ARG  | C-N   | 7.18  | 1.43        | 1.33     |
| 10  | C16   | 1782 | SER  | C-N   | -7.17 | 1.25        | 1.33     |
| 19  | 4     | 308  | GLU  | C-N   | -7.17 | 1.24        | 1.33     |
| 7   | Q16   | 227  | SER  | C-N   | -7.17 | 1.24        | 1.33     |
| 9   | K8    | 762  | SER  | C-N   | -7.17 | 1.24        | 1.33     |
| 22  | I24   | 114  | PRO  | N-CD  | -7.17 | 1.37        | 1.47     |
| 5   | P8    | 288  | ARG  | C-N   | -7.17 | 1.25        | 1.34     |
| 7   | Q16   | 86   | ALA  | C-N   | -7.17 | 1.24        | 1.32     |
| 10  | C16   | 1591 | LYS  | C-N   | 7.17  | 1.41        | 1.33     |
| 20  | E8    | 226  | CYS  | C-N   | -7.17 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 714  | GLY  | C-N   | 7.17  | 1.43        | 1.33     |
| 10  | C32   | 1591 | LYS  | C-N   | 7.17  | 1.41        | 1.33     |
| 10  | C16   | 606  | MET  | C-N   | -7.17 | 1.24        | 1.33     |
| 10  | C8    | 606  | MET  | C-N   | -7.17 | 1.24        | 1.33     |
| 10  | C32   | 1782 | SER  | C-N   | -7.17 | 1.25        | 1.33     |
| 9   | K     | 957  | ILE  | C-N   | -7.16 | 1.24        | 1.33     |
| 21  | H8    | 164  | ALA  | C-N   | -7.16 | 1.23        | 1.33     |
| 21  | H8    | 329  | LYS  | C-N   | -7.16 | 1.25        | 1.33     |
| 11  | A32   | 321  | ILE  | C-N   | -7.16 | 1.23        | 1.33     |
| 21  | H     | 241  | GLU  | C-N   | -7.16 | 1.24        | 1.33     |
| 5   | P16   | 288  | ARG  | C-N   | -7.16 | 1.25        | 1.34     |
| 10  | C16   | 1801 | SER  | C-N   | 7.16  | 1.43        | 1.34     |
| 10  | C24   | 1739 | VAL  | C-N   | -7.16 | 1.24        | 1.33     |
| 11  | A40   | 321  | ILE  | C-N   | -7.16 | 1.23        | 1.33     |
| 20  | E     | 226  | CYS  | C-N   | -7.16 | 1.24        | 1.33     |
| 10  | C24   | 553  | LEU  | C-N   | -7.15 | 1.24        | 1.33     |
| 10  | C     | 715  | PHE  | C-N   | 7.15  | 1.43        | 1.33     |
| 10  | C24   | 627  | VAL  | C-N   | 7.15  | 1.44        | 1.33     |
| 7   | Q8    | 227  | SER  | C-N   | -7.15 | 1.24        | 1.33     |
| 10  | C8    | 1348 | LEU  | C-N   | 7.15  | 1.43        | 1.34     |
| 6   | O     | 203  | ILE  | C-N   | -7.15 | 1.24        | 1.33     |
| 18  | B8    | 1213 | PRO  | N-CD  | -7.15 | 1.37        | 1.47     |
| 22  | I16   | 114  | PRO  | N-CD  | -7.15 | 1.37        | 1.47     |
| 18  | B     | 588  | PHE  | C-N   | 7.15  | 1.43        | 1.33     |
| 10  | C24   | 715  | PHE  | C-N   | 7.14  | 1.43        | 1.33     |
| 1   | R16   | 1397 | PHE  | C-N   | -7.14 | 1.24        | 1.33     |
| 10  | C16   | 714  | GLY  | C-N   | 7.14  | 1.43        | 1.33     |
| 10  | C24   | 1801 | SER  | C-N   | 7.14  | 1.43        | 1.34     |
| 20  | E     | 256  | ALA  | C-N   | -7.14 | 1.24        | 1.34     |
| 21  | H16   | 241  | GLU  | C-N   | -7.14 | 1.24        | 1.33     |
| 10  | C32   | 627  | VAL  | C-N   | 7.14  | 1.44        | 1.33     |
| 2   | M8    | 465  | GLY  | C-N   | 7.14  | 1.43        | 1.33     |
| 9   | K8    | 1106 | LEU  | C-N   | -7.14 | 1.24        | 1.34     |
| 10  | C16   | 344  | ASP  | C-N   | -7.14 | 1.24        | 1.33     |
| 11  | A16   | 321  | ILE  | C-N   | -7.14 | 1.23        | 1.33     |
| 18  | B     | 1896 | CYS  | C-N   | -7.14 | 1.24        | 1.33     |
| 20  | E     | 348  | PRO  | C-N   | -7.14 | 1.24        | 1.34     |
| 21  | H8    | 156  | GLU  | C-N   | -7.14 | 1.24        | 1.33     |
| 18  | B8    | 1896 | CYS  | C-N   | -7.13 | 1.24        | 1.33     |
| 21  | H24   | 156  | GLU  | C-N   | -7.13 | 1.24        | 1.33     |
| 11  | A16   | 323  | LEU  | C-N   | -7.13 | 1.24        | 1.34     |
| 21  | H     | 164  | ALA  | C-N   | -7.13 | 1.23        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | R     | 1397 | PHE  | C-N   | -7.13 | 1.24        | 1.33     |
| 18  | B8    | 1780 | LEU  | C-N   | -7.13 | 1.24        | 1.33     |
| 12  | A48   | 321  | ILE  | C-N   | -7.13 | 1.23        | 1.33     |
| 18  | B     | 1683 | THR  | C-N   | 7.13  | 1.43        | 1.33     |
| 19  | 4     | 13   | CYS  | C-N   | -7.13 | 1.24        | 1.33     |
| 21  | H16   | 156  | GLU  | C-N   | -7.13 | 1.24        | 1.33     |
| 5   | P     | 288  | ARG  | C-N   | -7.12 | 1.25        | 1.34     |
| 9   | K8    | 903  | ARG  | C-N   | -7.12 | 1.24        | 1.33     |
| 10  | C24   | 402  | ALA  | C-N   | -7.12 | 1.24        | 1.33     |
| 10  | C24   | 453  | LEU  | C-N   | 7.12  | 1.43        | 1.33     |
| 5   | P     | 599  | ASP  | C-N   | -7.12 | 1.24        | 1.33     |
| 10  | C8    | 1591 | LYS  | C-N   | 7.12  | 1.41        | 1.33     |
| 18  | B     | 1213 | PRO  | N-CD  | -7.12 | 1.37        | 1.47     |
| 19  | 4     | 8    | GLY  | C-N   | -7.12 | 1.23        | 1.33     |
| 9   | K     | 766  | GLU  | C-N   | -7.11 | 1.24        | 1.33     |
| 20  | E8    | 348  | PRO  | C-N   | -7.11 | 1.24        | 1.34     |
| 7   | Q16   | 254  | ALA  | C-N   | -7.11 | 1.24        | 1.33     |
| 10  | C     | 1801 | SER  | C-N   | 7.11  | 1.43        | 1.34     |
| 10  | C16   | 453  | LEU  | C-N   | 7.11  | 1.43        | 1.33     |
| 18  | B     | 1751 | CYS  | C-N   | -7.11 | 1.25        | 1.33     |
| 20  | E8    | 256  | ALA  | C-N   | -7.11 | 1.24        | 1.34     |
| 9   | K8    | 1173 | ASN  | C-N   | -7.10 | 1.24        | 1.34     |
| 10  | C24   | 1348 | LEU  | C-N   | 7.10  | 1.43        | 1.34     |
| 10  | C8    | 714  | GLY  | C-N   | 7.10  | 1.43        | 1.33     |
| 19  | 48    | 308  | GLU  | C-N   | -7.10 | 1.24        | 1.33     |
| 10  | C     | 714  | GLY  | C-N   | 7.10  | 1.43        | 1.33     |
| 10  | C8    | 453  | LEU  | C-N   | 7.10  | 1.43        | 1.33     |
| 6   | O8    | 149  | LEU  | C-N   | -7.10 | 1.24        | 1.33     |
| 9   | K8    | 810  | LEU  | C-N   | -7.10 | 1.24        | 1.33     |
| 10  | C     | 627  | VAL  | C-N   | 7.10  | 1.43        | 1.33     |
| 10  | C8    | 402  | ALA  | C-N   | -7.10 | 1.24        | 1.33     |
| 10  | C32   | 711  | ASP  | C-N   | 7.10  | 1.44        | 1.33     |
| 1   | R8    | 1397 | PHE  | C-N   | -7.10 | 1.24        | 1.33     |
| 9   | K8    | 766  | GLU  | C-N   | -7.10 | 1.24        | 1.33     |
| 9   | K8    | 1245 | GLU  | C-N   | -7.10 | 1.24        | 1.34     |
| 18  | B8    | 1683 | THR  | C-N   | 7.09  | 1.43        | 1.33     |
| 19  | 48    | 8    | GLY  | C-N   | -7.09 | 1.23        | 1.33     |
| 6   | O16   | 203  | ILE  | C-N   | -7.09 | 1.24        | 1.33     |
| 6   | O8    | 94   | GLY  | C-N   | -7.09 | 1.23        | 1.33     |
| 22  | I8    | 114  | PRO  | N-CD  | -7.09 | 1.37        | 1.47     |
| 10  | C     | 1782 | SER  | C-N   | -7.09 | 1.25        | 1.33     |
| 21  | H24   | 241  | GLU  | C-N   | -7.09 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A     | 323  | LEU  | C-N   | -7.08 | 1.24        | 1.34     |
| 22  | I     | 114  | PRO  | N-CD  | -7.08 | 1.37        | 1.47     |
| 10  | C8    | 1801 | SER  | C-N   | 7.08  | 1.43        | 1.34     |
| 18  | B     | 1924 | GLY  | C-N   | -7.08 | 1.23        | 1.33     |
| 2   | M16   | 800  | GLU  | C-N   | -7.08 | 1.24        | 1.33     |
| 10  | C32   | 402  | ALA  | C-N   | -7.08 | 1.24        | 1.33     |
| 12  | A     | 321  | ILE  | C-N   | -7.08 | 1.23        | 1.33     |
| 10  | C     | 402  | ALA  | C-N   | -7.08 | 1.24        | 1.33     |
| 18  | B     | 535  | ARG  | C-N   | 7.08  | 1.41        | 1.33     |
| 6   | O16   | 94   | GLY  | C-N   | -7.07 | 1.23        | 1.33     |
| 10  | C8    | 553  | LEU  | C-N   | -7.07 | 1.25        | 1.33     |
| 12  | A48   | 323  | LEU  | C-N   | -7.07 | 1.24        | 1.34     |
| 9   | K     | 1173 | ASN  | C-N   | -7.07 | 1.24        | 1.34     |
| 10  | C8    | 344  | ASP  | C-N   | -7.07 | 1.24        | 1.33     |
| 18  | B8    | 88   | LEU  | C-N   | -7.07 | 1.24        | 1.33     |
| 1   | R16   | 1220 | GLN  | C-N   | -7.07 | 1.25        | 1.33     |
| 22  | I8    | 198  | SER  | C-N   | -7.07 | 1.24        | 1.33     |
| 15  | J     | 618  | GLN  | C-N   | -7.06 | 1.24        | 1.33     |
| 18  | B8    | 1924 | GLY  | C-N   | -7.06 | 1.23        | 1.33     |
| 22  | I8    | 95   | LEU  | C-N   | -7.06 | 1.22        | 1.33     |
| 10  | C24   | 732  | THR  | C-N   | 7.06  | 1.43        | 1.33     |
| 10  | C     | 453  | LEU  | C-N   | 7.06  | 1.43        | 1.33     |
| 10  | C     | 711  | ASP  | C-N   | 7.06  | 1.44        | 1.33     |
| 6   | O     | 318  | GLN  | C-N   | -7.06 | 1.24        | 1.33     |
| 10  | C8    | 1067 | SER  | C-N   | 7.06  | 1.44        | 1.33     |
| 22  | I     | 198  | SER  | C-N   | -7.06 | 1.24        | 1.33     |
| 21  | H8    | 241  | GLU  | C-N   | -7.06 | 1.24        | 1.33     |
| 10  | C16   | 650  | ARG  | C-N   | 7.05  | 1.43        | 1.33     |
| 10  | C24   | 711  | ASP  | C-N   | 7.05  | 1.44        | 1.33     |
| 18  | B8    | 1889 | PRO  | N-CD  | -7.05 | 1.37        | 1.47     |
| 7   | Q     | 86   | ALA  | C-N   | -7.05 | 1.24        | 1.32     |
| 10  | C24   | 1782 | SER  | C-N   | -7.05 | 1.25        | 1.33     |
| 10  | C8    | 1782 | SER  | C-N   | -7.05 | 1.25        | 1.33     |
| 18  | B     | 1889 | PRO  | N-CD  | -7.05 | 1.37        | 1.47     |
| 18  | B8    | 479  | PRO  | N-CD  | 7.05  | 1.57        | 1.47     |
| 10  | C16   | 402  | ALA  | C-N   | -7.05 | 1.24        | 1.33     |
| 10  | C16   | 711  | ASP  | C-N   | 7.05  | 1.44        | 1.33     |
| 11  | A32   | 323  | LEU  | C-N   | -7.05 | 1.24        | 1.34     |
| 19  | 48    | 13   | CYS  | C-N   | -7.05 | 1.24        | 1.33     |
| 19  | 4     | 27   | ASP  | C-N   | -7.05 | 1.25        | 1.33     |
| 9   | K     | 903  | ARG  | C-N   | -7.04 | 1.25        | 1.33     |
| 2   | M16   | 260  | GLU  | C-N   | -7.04 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C     | 650  | ARG  | C-N   | 7.04  | 1.43        | 1.33     |
| 19  | 48    | 27   | ASP  | C-N   | -7.04 | 1.25        | 1.33     |
| 14  | W     | 773  | GLN  | C-N   | -7.04 | 1.23        | 1.33     |
| 10  | C16   | 767  | GLU  | C-N   | -7.04 | 1.24        | 1.34     |
| 2   | M8    | 800  | GLU  | C-N   | -7.04 | 1.24        | 1.33     |
| 18  | B8    | 1751 | CYS  | C-N   | -7.03 | 1.25        | 1.33     |
| 2   | M     | 674  | TYR  | C-N   | 7.03  | 1.43        | 1.33     |
| 20  | E     | 443  | ASP  | C-N   | -7.03 | 1.24        | 1.33     |
| 18  | B8    | 521  | PRO  | C-N   | -7.03 | 1.22        | 1.33     |
| 7   | Q8    | 86   | ALA  | C-N   | -7.03 | 1.24        | 1.32     |
| 10  | C24   | 997  | ILE  | C-N   | -7.03 | 1.23        | 1.33     |
| 11  | A40   | 323  | LEU  | C-N   | -7.03 | 1.24        | 1.34     |
| 10  | C8    | 711  | ASP  | C-N   | 7.03  | 1.44        | 1.33     |
| 18  | B     | 1857 | PRO  | N-CD  | -7.03 | 1.38        | 1.47     |
| 18  | B8    | 247  | GLY  | C-N   | 7.03  | 1.43        | 1.34     |
| 2   | M8    | 260  | GLU  | C-N   | -7.03 | 1.24        | 1.33     |
| 10  | C8    | 650  | ARG  | C-N   | 7.03  | 1.43        | 1.33     |
| 18  | B     | 88   | LEU  | C-N   | -7.03 | 1.24        | 1.33     |
| 18  | B     | 1596 | GLY  | C-N   | 7.03  | 1.43        | 1.33     |
| 18  | B8    | 535  | ARG  | C-N   | 7.03  | 1.41        | 1.33     |
| 22  | I16   | 95   | LEU  | C-N   | -7.03 | 1.23        | 1.33     |
| 10  | C32   | 453  | LEU  | C-N   | 7.03  | 1.43        | 1.33     |
| 10  | C32   | 1801 | SER  | C-N   | 7.03  | 1.43        | 1.34     |
| 6   | O16   | 318  | GLN  | C-N   | -7.02 | 1.24        | 1.33     |
| 10  | C16   | 553  | LEU  | C-N   | -7.02 | 1.25        | 1.33     |
| 10  | C32   | 650  | ARG  | C-N   | 7.02  | 1.43        | 1.33     |
| 20  | E     | 165  | ARG  | C-N   | -7.02 | 1.27        | 1.33     |
| 22  | I24   | 198  | SER  | C-N   | -7.02 | 1.24        | 1.33     |
| 10  | C16   | 732  | THR  | C-N   | 7.02  | 1.43        | 1.33     |
| 9   | K8    | 1284 | MET  | C-N   | 7.01  | 1.43        | 1.33     |
| 10  | C     | 997  | ILE  | C-N   | -7.01 | 1.23        | 1.33     |
| 22  | I24   | 107  | THR  | C-N   | 7.01  | 1.43        | 1.33     |
| 2   | M8    | 674  | TYR  | C-N   | 7.01  | 1.43        | 1.33     |
| 10  | C     | 553  | LEU  | C-N   | -7.00 | 1.25        | 1.33     |
| 10  | C32   | 1067 | SER  | C-N   | 7.00  | 1.44        | 1.33     |
| 9   | K     | 939  | ARG  | C-N   | -7.00 | 1.24        | 1.33     |
| 11  | A24   | 323  | LEU  | C-N   | -7.00 | 1.24        | 1.34     |
| 22  | I     | 107  | THR  | C-N   | 7.00  | 1.43        | 1.33     |
| 23  | J32   | 623  | GLU  | C-N   | -7.00 | 1.24        | 1.33     |
| 10  | C     | 325  | MET  | C-N   | -7.00 | 1.23        | 1.33     |
| 14  | W     | 659  | ARG  | C-N   | -7.00 | 1.24        | 1.33     |
| 10  | C     | 732  | THR  | C-N   | 7.00  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 247  | GLY  | C-N   | 7.00  | 1.43        | 1.34     |
| 18  | B     | 818  | SER  | C-N   | 7.00  | 1.43        | 1.33     |
| 10  | C32   | 1276 | SER  | C-N   | 7.00  | 1.45        | 1.33     |
| 11  | A24   | 856  | LYS  | C-N   | -6.99 | 1.25        | 1.33     |
| 1   | R8    | 1384 | LEU  | C-N   | -6.99 | 1.23        | 1.33     |
| 6   | O8    | 318  | GLN  | C-N   | -6.99 | 1.24        | 1.33     |
| 10  | C16   | 581  | TYR  | C-N   | -6.99 | 1.24        | 1.33     |
| 20  | E8    | 443  | ASP  | C-N   | -6.99 | 1.24        | 1.33     |
| 10  | C32   | 553  | LEU  | C-N   | -6.99 | 1.25        | 1.33     |
| 22  | I     | 95   | LEU  | C-N   | -6.99 | 1.23        | 1.33     |
| 3   | N8    | 42   | ASN  | C-N   | 6.99  | 1.43        | 1.33     |
| 6   | O     | 94   | GLY  | C-N   | -6.99 | 1.23        | 1.33     |
| 10  | C16   | 1545 | ARG  | C-N   | 6.99  | 1.43        | 1.33     |
| 10  | C24   | 1067 | SER  | C-N   | 6.99  | 1.44        | 1.33     |
| 2   | M     | 260  | GLU  | C-N   | -6.99 | 1.24        | 1.33     |
| 19  | 48    | 268  | TYR  | C-N   | -6.99 | 1.24        | 1.33     |
| 2   | M16   | 501  | ARG  | C-N   | 6.98  | 1.43        | 1.33     |
| 10  | C32   | 581  | TYR  | C-N   | -6.98 | 1.24        | 1.33     |
| 14  | W     | 787  | MET  | C-N   | -6.98 | 1.24        | 1.33     |
| 22  | I16   | 198  | SER  | C-N   | -6.98 | 1.24        | 1.33     |
| 1   | R     | 1384 | LEU  | C-N   | -6.98 | 1.23        | 1.33     |
| 10  | C16   | 997  | ILE  | C-N   | -6.98 | 1.23        | 1.33     |
| 10  | C16   | 1067 | SER  | C-N   | 6.98  | 1.44        | 1.33     |
| 10  | C     | 81   | LEU  | C-N   | -6.98 | 1.24        | 1.33     |
| 10  | C8    | 732  | THR  | C-N   | 6.98  | 1.43        | 1.33     |
| 22  | I16   | 107  | THR  | C-N   | 6.98  | 1.42        | 1.33     |
| 9   | K     | 1267 | LEU  | C-N   | -6.98 | 1.25        | 1.33     |
| 13  | V     | 924  | LYS  | C-N   | -6.98 | 1.23        | 1.33     |
| 10  | C8    | 1559 | HIS  | C-N   | -6.98 | 1.24        | 1.33     |
| 18  | B     | 521  | PRO  | C-N   | -6.98 | 1.22        | 1.33     |
| 2   | M16   | 408  | GLU  | C-N   | -6.98 | 1.24        | 1.33     |
| 14  | W     | 708  | PRO  | C-N   | -6.98 | 1.24        | 1.33     |
| 18  | B     | 479  | PRO  | N-CD  | 6.98  | 1.57        | 1.47     |
| 18  | B8    | 1857 | PRO  | N-CD  | -6.98 | 1.38        | 1.47     |
| 20  | E8    | 165  | ARG  | C-N   | -6.97 | 1.27        | 1.33     |
| 9   | K8    | 1261 | MET  | C-N   | -6.97 | 1.24        | 1.33     |
| 18  | B8    | 730  | GLU  | C-N   | -6.97 | 1.23        | 1.33     |
| 21  | H16   | 335  | LEU  | C-N   | 6.97  | 1.42        | 1.33     |
| 1   | R16   | 1384 | LEU  | C-N   | -6.97 | 1.23        | 1.33     |
| 3   | N16   | 42   | ASN  | C-N   | 6.96  | 1.43        | 1.33     |
| 9   | K8    | 939  | ARG  | C-N   | -6.96 | 1.24        | 1.33     |
| 9   | K8    | 1033 | GLN  | C-N   | -6.96 | 1.24        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 325  | MET  | C-N   | -6.96 | 1.23        | 1.33     |
| 3   | N     | 42   | ASN  | C-N   | 6.96  | 1.43        | 1.33     |
| 2   | M16   | 674  | TYR  | C-N   | 6.96  | 1.43        | 1.33     |
| 10  | C24   | 1276 | SER  | C-N   | 6.96  | 1.45        | 1.33     |
| 14  | W     | 652  | ILE  | C-N   | -6.96 | 1.25        | 1.33     |
| 10  | C     | 1067 | SER  | C-N   | 6.96  | 1.44        | 1.33     |
| 10  | C     | 1808 | ALA  | C-N   | 6.96  | 1.43        | 1.33     |
| 10  | C8    | 997  | ILE  | C-N   | -6.96 | 1.23        | 1.33     |
| 22  | I8    | 257  | LYS  | C-N   | 6.96  | 1.47        | 1.34     |
| 10  | C32   | 81   | LEU  | C-N   | -6.96 | 1.24        | 1.33     |
| 22  | I24   | 95   | LEU  | C-N   | -6.96 | 1.23        | 1.33     |
| 10  | C24   | 1545 | ARG  | C-N   | 6.96  | 1.43        | 1.33     |
| 19  | 4     | 268  | TYR  | C-N   | -6.96 | 1.24        | 1.33     |
| 10  | C32   | 325  | MET  | C-N   | -6.96 | 1.23        | 1.33     |
| 1   | R8    | 1227 | THR  | C-N   | -6.95 | 1.24        | 1.33     |
| 10  | C8    | 1203 | MET  | C-N   | 6.95  | 1.43        | 1.33     |
| 10  | C32   | 1006 | SER  | C-N   | -6.95 | 1.22        | 1.33     |
| 10  | C16   | 1099 | PRO  | N-CD  | -6.95 | 1.38        | 1.47     |
| 10  | C16   | 1006 | SER  | C-N   | -6.95 | 1.22        | 1.33     |
| 10  | C24   | 581  | TYR  | C-N   | -6.95 | 1.24        | 1.33     |
| 10  | C16   | 325  | MET  | C-N   | -6.95 | 1.23        | 1.33     |
| 12  | A     | 856  | LYS  | C-N   | -6.95 | 1.25        | 1.33     |
| 18  | B8    | 1283 | VAL  | C-N   | 6.95  | 1.42        | 1.33     |
| 12  | A48   | 856  | LYS  | C-N   | -6.95 | 1.25        | 1.33     |
| 10  | C8    | 977  | PRO  | C-N   | -6.94 | 1.24        | 1.33     |
| 18  | B     | 1623 | GLY  | C-N   | 6.94  | 1.43        | 1.34     |
| 20  | E     | 83   | VAL  | C-N   | -6.94 | 1.25        | 1.33     |
| 22  | I16   | 325  | ILE  | C-N   | -6.94 | 1.24        | 1.33     |
| 10  | C8    | 1006 | SER  | C-N   | -6.94 | 1.22        | 1.33     |
| 2   | M8    | 408  | GLU  | C-N   | -6.94 | 1.24        | 1.33     |
| 21  | H24   | 283  | LYS  | C-N   | -6.94 | 1.24        | 1.33     |
| 10  | C16   | 1808 | ALA  | C-N   | 6.94  | 1.43        | 1.33     |
| 11  | A40   | 856  | LYS  | C-N   | -6.94 | 1.25        | 1.33     |
| 13  | V     | 791  | GLN  | C-N   | -6.94 | 1.24        | 1.34     |
| 2   | M8    | 501  | ARG  | C-N   | 6.94  | 1.43        | 1.33     |
| 20  | E8    | 83   | VAL  | C-N   | -6.94 | 1.25        | 1.33     |
| 2   | M     | 800  | GLU  | C-N   | -6.93 | 1.24        | 1.33     |
| 9   | K     | 1284 | MET  | C-N   | 6.93  | 1.43        | 1.33     |
| 18  | B8    | 818  | SER  | C-N   | 6.93  | 1.43        | 1.33     |
| 22  | I8    | 107  | THR  | C-N   | 6.93  | 1.42        | 1.33     |
| 22  | I16   | 332  | MET  | C-N   | -6.93 | 1.24        | 1.33     |
| 13  | V     | 910  | GLU  | C-N   | -6.93 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C     | 1276 | SER  | C-N   | 6.93  | 1.45        | 1.33     |
| 18  | B     | 9    | SER  | C-N   | -6.93 | 1.23        | 1.33     |
| 18  | B     | 730  | GLU  | C-N   | -6.93 | 1.23        | 1.33     |
| 21  | H8    | 335  | LEU  | C-N   | 6.93  | 1.42        | 1.33     |
| 10  | C32   | 732  | THR  | C-N   | 6.93  | 1.43        | 1.33     |
| 10  | C8    | 1808 | ALA  | C-N   | 6.93  | 1.43        | 1.33     |
| 18  | B8    | 1596 | GLY  | C-N   | 6.93  | 1.43        | 1.33     |
| 1   | R     | 1220 | GLN  | C-N   | -6.93 | 1.25        | 1.33     |
| 9   | K     | 1261 | MET  | C-N   | -6.93 | 1.24        | 1.33     |
| 10  | C8    | 325  | MET  | C-N   | -6.93 | 1.23        | 1.33     |
| 18  | B     | 1786 | PRO  | C-N   | -6.93 | 1.24        | 1.33     |
| 10  | C32   | 1559 | HIS  | C-N   | -6.93 | 1.24        | 1.33     |
| 10  | C24   | 1559 | HIS  | C-N   | -6.92 | 1.24        | 1.33     |
| 10  | C32   | 1099 | PRO  | N-CD  | -6.92 | 1.38        | 1.47     |
| 1   | R16   | 1227 | THR  | C-N   | -6.92 | 1.24        | 1.33     |
| 10  | C16   | 1297 | HIS  | C-N   | -6.92 | 1.24        | 1.33     |
| 18  | B8    | 1786 | PRO  | C-N   | -6.92 | 1.24        | 1.33     |
| 10  | C16   | 81   | LEU  | C-N   | -6.92 | 1.24        | 1.33     |
| 23  | J24   | 623  | GLU  | C-N   | -6.92 | 1.24        | 1.33     |
| 22  | I16   | 257  | LYS  | C-N   | 6.92  | 1.47        | 1.34     |
| 23  | J16   | 623  | GLU  | C-N   | -6.92 | 1.24        | 1.33     |
| 21  | H8    | 326  | GLY  | C-N   | -6.92 | 1.24        | 1.33     |
| 9   | K8    | 583  | GLU  | C-N   | -6.91 | 1.24        | 1.34     |
| 21  | H24   | 335  | LEU  | C-N   | 6.91  | 1.42        | 1.33     |
| 7   | Q     | 256  | ASP  | C-N   | -6.91 | 1.24        | 1.33     |
| 9   | K     | 583  | GLU  | C-N   | -6.91 | 1.24        | 1.34     |
| 14  | W     | 623  | TYR  | C-N   | -6.91 | 1.25        | 1.33     |
| 18  | B8    | 9    | SER  | C-N   | -6.91 | 1.23        | 1.33     |
| 21  | H16   | 326  | GLY  | C-N   | -6.91 | 1.24        | 1.33     |
| 10  | C32   | 767  | GLU  | C-N   | -6.91 | 1.24        | 1.34     |
| 10  | C32   | 997  | ILE  | C-N   | -6.91 | 1.23        | 1.33     |
| 2   | M     | 353  | ILE  | C-N   | -6.91 | 1.24        | 1.33     |
| 10  | C     | 1006 | SER  | C-N   | -6.91 | 1.22        | 1.33     |
| 18  | B     | 1283 | VAL  | C-N   | 6.91  | 1.42        | 1.33     |
| 23  | J8    | 623  | GLU  | C-N   | -6.91 | 1.24        | 1.33     |
| 9   | K8    | 1267 | LEU  | C-N   | -6.91 | 1.25        | 1.33     |
| 14  | W     | 634  | TYR  | C-N   | -6.91 | 1.24        | 1.33     |
| 10  | C     | 767  | GLU  | C-N   | -6.91 | 1.24        | 1.34     |
| 10  | C16   | 1276 | SER  | C-N   | 6.91  | 1.45        | 1.33     |
| 2   | M8    | 353  | ILE  | C-N   | -6.90 | 1.24        | 1.33     |
| 10  | C16   | 1559 | HIS  | C-N   | -6.90 | 1.24        | 1.33     |
| 10  | C     | 603  | PHE  | C-N   | -6.90 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | H8    | 283  | LYS  | C-N   | -6.90 | 1.24        | 1.33     |
| 10  | C32   | 1545 | ARG  | C-N   | 6.90  | 1.43        | 1.33     |
| 10  | C32   | 1808 | ALA  | C-N   | 6.90  | 1.43        | 1.33     |
| 1   | R8    | 1220 | GLN  | C-N   | -6.90 | 1.25        | 1.33     |
| 9   | K8    | 732  | ALA  | C-N   | -6.90 | 1.24        | 1.33     |
| 18  | B8    | 1441 | LEU  | C-N   | 6.90  | 1.42        | 1.33     |
| 5   | P16   | 81   | GLY  | C-N   | 6.90  | 1.44        | 1.33     |
| 10  | C24   | 1006 | SER  | C-N   | -6.90 | 1.22        | 1.33     |
| 10  | C24   | 81   | LEU  | C-N   | -6.90 | 1.24        | 1.33     |
| 22  | I24   | 257  | LYS  | C-N   | 6.90  | 1.47        | 1.34     |
| 21  | H16   | 313  | ALA  | C-N   | -6.90 | 1.23        | 1.33     |
| 10  | C     | 1297 | HIS  | C-N   | -6.90 | 1.24        | 1.33     |
| 21  | H     | 326  | GLY  | C-N   | -6.90 | 1.24        | 1.33     |
| 21  | H16   | 347  | GLU  | C-N   | -6.90 | 1.24        | 1.33     |
| 10  | C     | 1803 | THR  | C-N   | -6.89 | 1.25        | 1.33     |
| 10  | C32   | 1069 | TYR  | C-N   | 6.89  | 1.41        | 1.33     |
| 6   | O16   | 196  | PRO  | C-N   | -6.89 | 1.24        | 1.33     |
| 10  | C     | 977  | PRO  | C-N   | -6.89 | 1.24        | 1.33     |
| 11  | A16   | 856  | LYS  | C-N   | -6.89 | 1.25        | 1.33     |
| 22  | I24   | 332  | MET  | C-N   | -6.89 | 1.25        | 1.33     |
| 20  | E     | 339  | LYS  | C-N   | -6.89 | 1.23        | 1.33     |
| 22  | I     | 204  | PRO  | C-N   | -6.89 | 1.23        | 1.33     |
| 10  | C8    | 1276 | SER  | C-N   | 6.89  | 1.45        | 1.33     |
| 21  | H8    | 347  | GLU  | C-N   | -6.89 | 1.24        | 1.33     |
| 22  | I8    | 204  | PRO  | C-N   | -6.89 | 1.23        | 1.33     |
| 6   | O     | 196  | PRO  | C-N   | -6.88 | 1.24        | 1.33     |
| 10  | C24   | 1808 | ALA  | C-N   | 6.88  | 1.43        | 1.33     |
| 10  | C32   | 603  | PHE  | C-N   | -6.88 | 1.25        | 1.33     |
| 10  | C32   | 977  | PRO  | C-N   | -6.88 | 1.24        | 1.33     |
| 10  | C32   | 1280 | VAL  | C-N   | -6.88 | 1.23        | 1.33     |
| 7   | Q8    | 216  | GLN  | C-N   | -6.88 | 1.23        | 1.33     |
| 10  | C     | 1420 | LEU  | C-N   | 6.88  | 1.43        | 1.33     |
| 18  | B8    | 275  | LEU  | C-N   | -6.88 | 1.25        | 1.33     |
| 22  | I     | 257  | LYS  | C-N   | 6.88  | 1.47        | 1.34     |
| 10  | C32   | 1203 | MET  | C-N   | 6.88  | 1.43        | 1.33     |
| 10  | C     | 1099 | PRO  | N-CD  | -6.88 | 1.38        | 1.47     |
| 21  | H16   | 316  | ILE  | C-N   | -6.88 | 1.24        | 1.33     |
| 11  | A40   | 391  | GLU  | C-N   | -6.88 | 1.25        | 1.33     |
| 10  | C8    | 1069 | TYR  | C-N   | 6.88  | 1.41        | 1.33     |
| 22  | I     | 332  | MET  | C-N   | -6.88 | 1.25        | 1.33     |
| 22  | I8    | 325  | ILE  | C-N   | -6.88 | 1.25        | 1.33     |
| 10  | C16   | 603  | PHE  | C-N   | -6.88 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1297 | HIS  | C-N   | -6.88 | 1.24        | 1.33     |
| 20  | E8    | 483  | SER  | C-N   | -6.88 | 1.24        | 1.33     |
| 1   | R     | 1231 | MET  | C-N   | -6.88 | 1.24        | 1.33     |
| 10  | C8    | 1297 | HIS  | C-N   | -6.88 | 1.24        | 1.33     |
| 7   | Q8    | 256  | ASP  | C-N   | -6.87 | 1.24        | 1.33     |
| 10  | C32   | 1318 | ARG  | C-N   | -6.87 | 1.24        | 1.33     |
| 10  | C     | 1559 | HIS  | C-N   | -6.87 | 1.25        | 1.33     |
| 18  | B8    | 1623 | GLY  | C-N   | 6.87  | 1.43        | 1.34     |
| 21  | H     | 335  | LEU  | C-N   | 6.87  | 1.42        | 1.33     |
| 10  | C32   | 1297 | HIS  | C-N   | -6.87 | 1.24        | 1.33     |
| 10  | C     | 1203 | MET  | C-N   | 6.87  | 1.43        | 1.33     |
| 21  | H     | 347  | GLU  | C-N   | -6.87 | 1.24        | 1.33     |
| 2   | M     | 501  | ARG  | C-N   | 6.87  | 1.43        | 1.33     |
| 2   | M16   | 353  | ILE  | C-N   | -6.87 | 1.24        | 1.33     |
| 10  | C8    | 1545 | ARG  | C-N   | 6.87  | 1.43        | 1.33     |
| 7   | Q16   | 256  | ASP  | C-N   | -6.87 | 1.24        | 1.33     |
| 22  | I24   | 325  | ILE  | C-N   | -6.87 | 1.25        | 1.33     |
| 10  | C24   | 1099 | PRO  | N-CD  | -6.86 | 1.38        | 1.47     |
| 10  | C     | 581  | TYR  | C-N   | -6.86 | 1.24        | 1.33     |
| 10  | C8    | 1099 | PRO  | N-CD  | -6.86 | 1.38        | 1.47     |
| 18  | B     | 1043 | PRO  | N-CD  | -6.86 | 1.38        | 1.47     |
| 10  | C24   | 1280 | VAL  | C-N   | -6.86 | 1.23        | 1.33     |
| 10  | C     | 1280 | VAL  | C-N   | -6.86 | 1.23        | 1.33     |
| 20  | E     | 483  | SER  | C-N   | -6.86 | 1.24        | 1.33     |
| 9   | K8    | 877  | GLU  | C-N   | -6.86 | 1.25        | 1.33     |
| 18  | B     | 1441 | LEU  | C-N   | 6.86  | 1.42        | 1.33     |
| 21  | H24   | 347  | GLU  | C-N   | -6.86 | 1.24        | 1.33     |
| 1   | R     | 1227 | THR  | C-N   | -6.85 | 1.25        | 1.33     |
| 10  | C8    | 81   | LEU  | C-N   | -6.85 | 1.24        | 1.33     |
| 22  | I16   | 204  | PRO  | C-N   | -6.85 | 1.23        | 1.33     |
| 10  | C8    | 1280 | VAL  | C-N   | -6.85 | 1.23        | 1.33     |
| 18  | B8    | 1043 | PRO  | N-CD  | -6.85 | 1.38        | 1.47     |
| 9   | K     | 1033 | GLN  | C-N   | -6.85 | 1.24        | 1.34     |
| 10  | C16   | 1069 | TYR  | C-N   | 6.85  | 1.41        | 1.33     |
| 2   | M     | 408  | GLU  | C-N   | -6.85 | 1.24        | 1.33     |
| 6   | O8    | 196  | PRO  | C-N   | -6.84 | 1.24        | 1.33     |
| 21  | H24   | 326  | GLY  | C-N   | -6.84 | 1.24        | 1.33     |
| 10  | C8    | 767  | GLU  | C-N   | -6.84 | 1.24        | 1.34     |
| 1   | R8    | 1231 | MET  | C-N   | -6.84 | 1.24        | 1.33     |
| 1   | R16   | 1231 | MET  | C-N   | -6.84 | 1.24        | 1.33     |
| 12  | A48   | 391  | GLU  | C-N   | -6.84 | 1.25        | 1.33     |
| 1   | R     | 1445 | GLU  | C-N   | -6.84 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | I     | 325  | ILE  | C-N   | -6.84 | 1.25        | 1.33     |
| 13  | V     | 851  | THR  | C-N   | -6.84 | 1.25        | 1.33     |
| 21  | H8    | 313  | ALA  | C-N   | -6.84 | 1.23        | 1.33     |
| 21  | H8    | 316  | ILE  | C-N   | -6.84 | 1.24        | 1.33     |
| 21  | H16   | 217  | ARG  | C-N   | -6.83 | 1.25        | 1.33     |
| 10  | C24   | 1176 | VAL  | C-N   | -6.83 | 1.25        | 1.33     |
| 18  | B     | 1900 | ILE  | C-N   | -6.83 | 1.24        | 1.33     |
| 10  | C24   | 125  | THR  | C-N   | 6.83  | 1.42        | 1.33     |
| 11  | A32   | 153  | ARG  | C-N   | -6.83 | 1.26        | 1.33     |
| 10  | C32   | 1803 | THR  | C-N   | -6.83 | 1.25        | 1.33     |
| 1   | R16   | 1423 | SER  | C-N   | -6.83 | 1.24        | 1.33     |
| 11  | A24   | 391  | GLU  | C-N   | -6.83 | 1.25        | 1.33     |
| 14  | W     | 609  | THR  | C-N   | -6.83 | 1.25        | 1.33     |
| 10  | C8    | 603  | PHE  | C-N   | -6.83 | 1.25        | 1.33     |
| 5   | P     | 391  | LYS  | C-N   | 6.83  | 1.49        | 1.33     |
| 7   | Q     | 216  | GLN  | C-N   | -6.83 | 1.23        | 1.33     |
| 9   | K     | 1061 | GLY  | C-N   | 6.83  | 1.49        | 1.33     |
| 5   | P16   | 391  | LYS  | C-N   | 6.83  | 1.49        | 1.33     |
| 11  | A16   | 391  | GLU  | C-N   | -6.83 | 1.25        | 1.33     |
| 19  | 4     | 235  | SER  | C-N   | -6.82 | 1.24        | 1.33     |
| 19  | 48    | 235  | SER  | C-N   | -6.82 | 1.24        | 1.33     |
| 22  | I8    | 332  | MET  | C-N   | -6.82 | 1.25        | 1.33     |
| 22  | I24   | 204  | PRO  | C-N   | -6.82 | 1.23        | 1.33     |
| 15  | J     | 622  | GLU  | C-N   | -6.82 | 1.24        | 1.33     |
| 23  | J8    | 723  | GLN  | C-N   | 6.82  | 1.39        | 1.33     |
| 2   | M     | 386  | ASN  | C-N   | 6.82  | 1.43        | 1.33     |
| 5   | P8    | 81   | GLY  | C-N   | 6.82  | 1.44        | 1.33     |
| 10  | C16   | 1814 | LYS  | C-N   | -6.82 | 1.25        | 1.33     |
| 1   | R8    | 1423 | SER  | C-N   | -6.82 | 1.24        | 1.33     |
| 7   | Q16   | 123  | GLU  | C-N   | -6.82 | 1.24        | 1.33     |
| 7   | Q16   | 216  | GLN  | C-N   | -6.82 | 1.23        | 1.33     |
| 13  | V     | 765  | ASN  | C-N   | -6.82 | 1.24        | 1.33     |
| 10  | C8    | 1318 | ARG  | C-N   | -6.82 | 1.24        | 1.33     |
| 2   | M8    | 386  | ASN  | C-N   | 6.82  | 1.43        | 1.33     |
| 9   | K8    | 1061 | GLY  | C-N   | 6.82  | 1.49        | 1.33     |
| 10  | C8    | 581  | TYR  | C-N   | -6.82 | 1.24        | 1.33     |
| 21  | H24   | 217  | ARG  | C-N   | -6.82 | 1.25        | 1.33     |
| 20  | E     | 34   | ASN  | C-N   | -6.81 | 1.25        | 1.33     |
| 11  | A16   | 153  | ARG  | C-N   | -6.81 | 1.26        | 1.33     |
| 11  | A32   | 856  | LYS  | C-N   | -6.81 | 1.25        | 1.33     |
| 7   | Q     | 6    | ASP  | C-N   | 6.81  | 1.43        | 1.33     |
| 9   | K     | 732  | ALA  | C-N   | -6.81 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 977  | PRO  | C-N   | -6.81 | 1.24        | 1.33     |
| 10  | C16   | 1176 | VAL  | C-N   | -6.81 | 1.25        | 1.33     |
| 10  | C16   | 1280 | VAL  | C-N   | -6.81 | 1.23        | 1.33     |
| 10  | C24   | 603  | PHE  | C-N   | -6.81 | 1.25        | 1.33     |
| 10  | C24   | 767  | GLU  | C-N   | -6.81 | 1.24        | 1.34     |
| 18  | B     | 35   | PRO  | C-N   | -6.81 | 1.25        | 1.33     |
| 21  | H     | 224  | ASN  | C-N   | -6.81 | 1.25        | 1.33     |
| 18  | B8    | 245  | LEU  | C-N   | 6.80  | 1.44        | 1.33     |
| 10  | C32   | 1176 | VAL  | C-N   | -6.80 | 1.25        | 1.33     |
| 1   | R8    | 1445 | GLU  | C-N   | -6.80 | 1.24        | 1.33     |
| 10  | C24   | 1814 | LYS  | C-N   | -6.80 | 1.25        | 1.33     |
| 21  | H8    | 203  | ARG  | C-N   | -6.80 | 1.25        | 1.33     |
| 13  | V     | 784  | LYS  | C-N   | -6.80 | 1.24        | 1.33     |
| 18  | B8    | 1473 | SER  | C-N   | 6.80  | 1.43        | 1.33     |
| 21  | H     | 283  | LYS  | C-N   | -6.80 | 1.24        | 1.33     |
| 5   | P8    | 391  | LYS  | C-N   | 6.80  | 1.49        | 1.33     |
| 18  | B     | 275  | LEU  | C-N   | -6.80 | 1.25        | 1.33     |
| 5   | P     | 81   | GLY  | C-N   | 6.79  | 1.44        | 1.33     |
| 14  | W     | 736  | GLU  | C-N   | -6.79 | 1.24        | 1.33     |
| 5   | P8    | 209  | THR  | C-N   | -6.79 | 1.25        | 1.34     |
| 9   | K8    | 792  | LEU  | C-N   | -6.79 | 1.24        | 1.33     |
| 20  | E8    | 339  | LYS  | C-N   | -6.79 | 1.23        | 1.33     |
| 21  | H24   | 203  | ARG  | C-N   | -6.79 | 1.25        | 1.33     |
| 21  | H16   | 283  | LYS  | C-N   | -6.79 | 1.24        | 1.33     |
| 10  | C16   | 125  | THR  | C-N   | 6.79  | 1.42        | 1.33     |
| 10  | C8    | 1803 | THR  | C-N   | -6.79 | 1.25        | 1.33     |
| 18  | B     | 1473 | SER  | C-N   | 6.79  | 1.43        | 1.33     |
| 20  | E     | 158  | LEU  | C-N   | -6.79 | 1.24        | 1.33     |
| 19  | 48    | 351  | GLY  | C-N   | -6.79 | 1.24        | 1.33     |
| 21  | H24   | 313  | ALA  | C-N   | -6.79 | 1.23        | 1.33     |
| 10  | C16   | 1420 | LEU  | C-N   | 6.79  | 1.42        | 1.33     |
| 10  | C24   | 977  | PRO  | C-N   | -6.79 | 1.24        | 1.33     |
| 21  | H24   | 224  | ASN  | C-N   | -6.79 | 1.25        | 1.33     |
| 10  | C     | 1318 | ARG  | C-N   | -6.79 | 1.24        | 1.33     |
| 18  | B     | 1798 | VAL  | C-N   | 6.79  | 1.42        | 1.33     |
| 1   | R     | 1423 | SER  | C-N   | -6.79 | 1.24        | 1.33     |
| 10  | C     | 1069 | TYR  | C-N   | 6.79  | 1.41        | 1.33     |
| 10  | C16   | 1318 | ARG  | C-N   | -6.78 | 1.24        | 1.33     |
| 18  | B     | 245  | LEU  | C-N   | 6.78  | 1.43        | 1.33     |
| 19  | 4     | 94   | VAL  | C-N   | -6.78 | 1.24        | 1.34     |
| 5   | P8    | 392  | PRO  | C-N   | -6.78 | 1.20        | 1.33     |
| 12  | A     | 391  | GLU  | C-N   | -6.78 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | P8    | 541  | ARG  | C-N   | -6.78 | 1.24        | 1.33     |
| 21  | H     | 313  | ALA  | C-N   | -6.78 | 1.23        | 1.33     |
| 2   | M16   | 386  | ASN  | C-N   | 6.78  | 1.43        | 1.33     |
| 10  | C16   | 1803 | THR  | C-N   | -6.78 | 1.25        | 1.33     |
| 10  | C32   | 1310 | HIS  | C-N   | 6.78  | 1.43        | 1.33     |
| 10  | C32   | 1420 | LEU  | C-N   | 6.78  | 1.42        | 1.33     |
| 7   | Q8    | 123  | GLU  | C-N   | -6.77 | 1.24        | 1.33     |
| 9   | K     | 877  | GLU  | C-N   | -6.77 | 1.25        | 1.33     |
| 10  | C32   | 843  | MET  | C-N   | -6.77 | 1.24        | 1.33     |
| 10  | C32   | 125  | THR  | C-N   | 6.77  | 1.42        | 1.33     |
| 1   | R16   | 1445 | GLU  | C-N   | -6.77 | 1.24        | 1.33     |
| 10  | C8    | 1310 | HIS  | C-N   | 6.77  | 1.43        | 1.33     |
| 10  | C24   | 1069 | TYR  | C-N   | 6.76  | 1.41        | 1.33     |
| 10  | C24   | 1189 | LYS  | C-N   | -6.76 | 1.25        | 1.33     |
| 5   | P8    | 593  | GLN  | C-N   | -6.76 | 1.25        | 1.34     |
| 10  | C16   | 843  | MET  | C-N   | -6.76 | 1.24        | 1.33     |
| 2   | M     | 508  | ASN  | C-N   | 6.76  | 1.43        | 1.33     |
| 7   | Q16   | 190  | PRO  | N-CD  | 6.76  | 1.57        | 1.47     |
| 12  | A     | 237  | LEU  | C-N   | -6.76 | 1.23        | 1.33     |
| 21  | H     | 316  | ILE  | C-N   | -6.76 | 1.24        | 1.33     |
| 21  | H24   | 316  | ILE  | C-N   | -6.76 | 1.24        | 1.33     |
| 10  | C32   | 251  | GLY  | C-N   | -6.76 | 1.24        | 1.33     |
| 18  | B     | 912  | ILE  | C-N   | 6.76  | 1.43        | 1.33     |
| 19  | 4     | 29   | ARG  | C-N   | -6.76 | 1.25        | 1.33     |
| 19  | 48    | 94   | VAL  | C-N   | -6.76 | 1.25        | 1.34     |
| 9   | K     | 703  | LEU  | C-N   | -6.76 | 1.25        | 1.33     |
| 11  | A32   | 391  | GLU  | C-N   | -6.76 | 1.25        | 1.33     |
| 19  | 4     | 351  | GLY  | C-N   | -6.76 | 1.24        | 1.33     |
| 10  | C16   | 1203 | MET  | C-N   | 6.75  | 1.42        | 1.33     |
| 21  | H     | 203  | ARG  | C-N   | -6.75 | 1.25        | 1.33     |
| 10  | C8    | 678  | ARG  | C-N   | -6.75 | 1.24        | 1.33     |
| 5   | P     | 392  | PRO  | C-N   | -6.75 | 1.20        | 1.33     |
| 7   | Q     | 123  | GLU  | C-N   | -6.75 | 1.24        | 1.33     |
| 5   | P16   | 392  | PRO  | C-N   | -6.75 | 1.20        | 1.33     |
| 10  | C     | 125  | THR  | C-N   | 6.75  | 1.42        | 1.33     |
| 21  | H     | 217  | ARG  | C-N   | -6.75 | 1.25        | 1.33     |
| 12  | A48   | 237  | LEU  | C-N   | -6.75 | 1.23        | 1.33     |
| 5   | P     | 593  | GLN  | C-N   | -6.75 | 1.25        | 1.34     |
| 23  | J16   | 723  | GLN  | C-N   | 6.75  | 1.39        | 1.33     |
| 10  | C32   | 1753 | THR  | C-N   | -6.75 | 1.24        | 1.33     |
| 22  | I     | 143  | LEU  | C-N   | 6.74  | 1.44        | 1.33     |
| 2   | M     | 254  | LEU  | C-N   | 6.74  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K8    | 703  | LEU  | C-N   | -6.74 | 1.25        | 1.33     |
| 10  | C24   | 1310 | HIS  | C-N   | 6.74  | 1.43        | 1.33     |
| 15  | J     | 561  | PHE  | C-N   | -6.74 | 1.25        | 1.33     |
| 18  | B8    | 1900 | ILE  | C-N   | -6.74 | 1.24        | 1.33     |
| 7   | Q8    | 172  | LYS  | C-N   | -6.74 | 1.25        | 1.33     |
| 14  | W     | 742  | VAL  | C-N   | -6.74 | 1.24        | 1.33     |
| 10  | C     | 1176 | VAL  | C-N   | -6.74 | 1.25        | 1.33     |
| 19  | 48    | 31   | GLN  | C-N   | -6.74 | 1.24        | 1.34     |
| 22  | I24   | 99   | ASP  | C-N   | 6.74  | 1.43        | 1.33     |
| 2   | M8    | 508  | ASN  | C-N   | 6.74  | 1.43        | 1.33     |
| 15  | J     | 666  | ARG  | C-N   | -6.74 | 1.24        | 1.33     |
| 10  | C8    | 251  | GLY  | C-N   | -6.74 | 1.24        | 1.33     |
| 10  | C     | 843  | MET  | C-N   | -6.74 | 1.24        | 1.33     |
| 11  | A24   | 309  | VAL  | C-N   | -6.73 | 1.26        | 1.33     |
| 19  | 48    | 29   | ARG  | C-N   | -6.73 | 1.25        | 1.33     |
| 21  | H8    | 217  | ARG  | C-N   | -6.73 | 1.25        | 1.33     |
| 2   | M16   | 508  | ASN  | C-N   | 6.73  | 1.43        | 1.33     |
| 10  | C8    | 1630 | LEU  | C-N   | -6.73 | 1.25        | 1.33     |
| 10  | C8    | 1814 | LYS  | C-N   | -6.73 | 1.25        | 1.33     |
| 5   | P     | 574  | SER  | C-N   | -6.73 | 1.25        | 1.33     |
| 11  | A16   | 414  | ALA  | C-N   | -6.73 | 1.24        | 1.33     |
| 7   | Q8    | 6    | ASP  | C-N   | 6.73  | 1.43        | 1.33     |
| 22  | I8    | 143  | LEU  | C-N   | 6.73  | 1.44        | 1.33     |
| 21  | H16   | 224  | ASN  | C-N   | -6.73 | 1.25        | 1.33     |
| 10  | C16   | 1189 | LYS  | C-N   | -6.72 | 1.25        | 1.33     |
| 18  | B8    | 912  | ILE  | C-N   | 6.72  | 1.43        | 1.33     |
| 20  | E8    | 158  | LEU  | C-N   | -6.72 | 1.24        | 1.33     |
| 18  | B8    | 35   | PRO  | C-N   | -6.72 | 1.25        | 1.33     |
| 10  | C     | 1630 | LEU  | C-N   | -6.72 | 1.25        | 1.33     |
| 20  | E8    | 34   | ASN  | C-N   | -6.72 | 1.25        | 1.33     |
| 11  | A24   | 853  | LEU  | C-N   | -6.72 | 1.25        | 1.33     |
| 11  | A16   | 237  | LEU  | C-N   | -6.72 | 1.23        | 1.33     |
| 18  | B     | 1610 | LEU  | C-N   | 6.72  | 1.42        | 1.33     |
| 18  | B8    | 1610 | LEU  | C-N   | 6.72  | 1.42        | 1.33     |
| 5   | P16   | 593  | GLN  | C-N   | -6.72 | 1.25        | 1.34     |
| 21  | H16   | 203  | ARG  | C-N   | -6.72 | 1.25        | 1.33     |
| 9   | K8    | 1015 | ILE  | C-N   | -6.72 | 1.24        | 1.33     |
| 10  | C8    | 843  | MET  | C-N   | -6.72 | 1.24        | 1.33     |
| 10  | C24   | 1318 | ARG  | C-N   | -6.71 | 1.24        | 1.33     |
| 10  | C32   | 1630 | LEU  | C-N   | -6.71 | 1.25        | 1.33     |
| 5   | P16   | 574  | SER  | C-N   | -6.71 | 1.25        | 1.33     |
| 9   | K8    | 595  | PHE  | C-N   | -6.71 | 1.24        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A24   | 237  | LEU  | C-N   | -6.71 | 1.23        | 1.33     |
| 14  | W     | 683  | LYS  | C-N   | -6.71 | 1.24        | 1.33     |
| 18  | B8    | 1798 | VAL  | C-N   | 6.71  | 1.42        | 1.33     |
| 22  | I8    | 99   | ASP  | C-N   | 6.71  | 1.43        | 1.33     |
| 10  | C24   | 880  | GLU  | C-N   | 6.71  | 1.43        | 1.33     |
| 10  | C24   | 1803 | THR  | C-N   | -6.71 | 1.25        | 1.33     |
| 19  | 4     | 154  | PRO  | C-N   | -6.71 | 1.24        | 1.33     |
| 10  | C24   | 642  | GLU  | C-N   | -6.70 | 1.25        | 1.33     |
| 10  | C24   | 1203 | MET  | C-N   | 6.70  | 1.42        | 1.33     |
| 12  | A     | 853  | LEU  | C-N   | -6.70 | 1.25        | 1.33     |
| 10  | C8    | 1176 | VAL  | C-N   | -6.70 | 1.25        | 1.33     |
| 11  | A32   | 414  | ALA  | C-N   | -6.70 | 1.24        | 1.33     |
| 19  | 48    | 154  | PRO  | C-N   | -6.70 | 1.24        | 1.33     |
| 5   | P16   | 209  | THR  | C-N   | -6.70 | 1.25        | 1.34     |
| 10  | C8    | 642  | GLU  | C-N   | -6.70 | 1.25        | 1.33     |
| 23  | J24   | 723  | GLN  | C-N   | 6.70  | 1.39        | 1.33     |
| 10  | C32   | 1814 | LYS  | C-N   | -6.70 | 1.25        | 1.33     |
| 9   | K     | 595  | PHE  | C-N   | -6.69 | 1.24        | 1.34     |
| 9   | K8    | 881  | GLY  | C-N   | -6.69 | 1.24        | 1.33     |
| 10  | C8    | 125  | THR  | C-N   | 6.69  | 1.42        | 1.33     |
| 23  | J32   | 593  | VAL  | C-N   | -6.69 | 1.25        | 1.33     |
| 23  | J32   | 723  | GLN  | C-N   | 6.69  | 1.39        | 1.33     |
| 21  | H8    | 224  | ASN  | C-N   | -6.69 | 1.25        | 1.33     |
| 10  | C32   | 678  | ARG  | C-N   | -6.69 | 1.24        | 1.33     |
| 5   | P     | 209  | THR  | C-N   | -6.69 | 1.25        | 1.34     |
| 10  | C24   | 1420 | LEU  | C-N   | 6.69  | 1.42        | 1.33     |
| 14  | W     | 593  | GLY  | C-N   | 6.69  | 1.41        | 1.33     |
| 10  | C32   | 1189 | LYS  | C-N   | -6.69 | 1.25        | 1.33     |
| 3   | N8    | 281  | ASN  | C-N   | 6.69  | 1.43        | 1.33     |
| 10  | C16   | 678  | ARG  | C-N   | -6.69 | 1.24        | 1.33     |
| 10  | C16   | 1310 | HIS  | C-N   | 6.69  | 1.43        | 1.33     |
| 10  | C     | 678  | ARG  | C-N   | -6.69 | 1.24        | 1.33     |
| 7   | Q16   | 172  | LYS  | C-N   | -6.69 | 1.25        | 1.33     |
| 10  | C8    | 1420 | LEU  | C-N   | 6.69  | 1.42        | 1.33     |
| 3   | N16   | 281  | ASN  | C-N   | 6.68  | 1.43        | 1.33     |
| 12  | A     | 414  | ALA  | C-N   | -6.68 | 1.24        | 1.33     |
| 14  | W     | 765  | LYS  | C-N   | 6.68  | 1.43        | 1.33     |
| 19  | 4     | 31   | GLN  | C-N   | -6.68 | 1.24        | 1.34     |
| 9   | K     | 792  | LEU  | C-N   | -6.68 | 1.24        | 1.33     |
| 10  | C     | 1430 | ARG  | C-N   | -6.68 | 1.25        | 1.33     |
| 10  | C     | 1753 | THR  | C-N   | -6.68 | 1.24        | 1.33     |
| 19  | 48    | 375  | ASP  | C-N   | -6.68 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A24   | 414  | ALA  | C-N   | -6.68 | 1.24        | 1.33     |
| 10  | C     | 642  | GLU  | C-N   | -6.68 | 1.25        | 1.33     |
| 10  | C32   | 642  | GLU  | C-N   | -6.68 | 1.25        | 1.33     |
| 10  | C16   | 984  | SER  | C-N   | -6.68 | 1.25        | 1.33     |
| 15  | J     | 676  | GLN  | C-N   | 6.68  | 1.43        | 1.33     |
| 7   | Q16   | 57   | ASN  | C-N   | -6.68 | 1.25        | 1.33     |
| 7   | Q16   | 6    | ASP  | C-N   | 6.68  | 1.43        | 1.33     |
| 10  | C8    | 1753 | THR  | C-N   | -6.68 | 1.24        | 1.33     |
| 10  | C16   | 1753 | THR  | C-N   | -6.67 | 1.24        | 1.33     |
| 10  | C     | 1814 | LYS  | C-N   | -6.67 | 1.25        | 1.33     |
| 18  | B     | 1475 | SER  | C-N   | 6.67  | 1.43        | 1.33     |
| 22  | I24   | 143  | LEU  | C-N   | 6.67  | 1.44        | 1.33     |
| 10  | C16   | 642  | GLU  | C-N   | -6.67 | 1.25        | 1.33     |
| 22  | I     | 99   | ASP  | C-N   | 6.67  | 1.42        | 1.33     |
| 10  | C24   | 843  | MET  | C-N   | -6.67 | 1.24        | 1.33     |
| 11  | A40   | 414  | ALA  | C-N   | -6.67 | 1.24        | 1.33     |
| 18  | B     | 1098 | MET  | C-N   | -6.67 | 1.25        | 1.33     |
| 19  | 48    | 34   | TYR  | C-N   | -6.67 | 1.25        | 1.33     |
| 12  | A48   | 309  | VAL  | C-N   | -6.67 | 1.26        | 1.33     |
| 9   | K     | 660  | GLN  | C-N   | -6.67 | 1.24        | 1.33     |
| 15  | J     | 584  | ARG  | C-N   | -6.67 | 1.24        | 1.33     |
| 11  | A16   | 309  | VAL  | C-N   | -6.67 | 1.26        | 1.33     |
| 10  | C16   | 251  | GLY  | C-N   | -6.67 | 1.24        | 1.33     |
| 10  | C24   | 678  | ARG  | C-N   | -6.67 | 1.24        | 1.33     |
| 13  | V     | 824  | TRP  | C-N   | -6.67 | 1.25        | 1.33     |
| 22  | I16   | 99   | ASP  | C-N   | 6.67  | 1.42        | 1.33     |
| 12  | A48   | 414  | ALA  | C-N   | -6.67 | 1.25        | 1.33     |
| 2   | M8    | 254  | LEU  | C-N   | 6.67  | 1.42        | 1.33     |
| 7   | Q     | 57   | ASN  | C-N   | -6.67 | 1.25        | 1.33     |
| 18  | B8    | 1911 | LEU  | C-N   | -6.67 | 1.25        | 1.33     |
| 5   | P8    | 574  | SER  | C-N   | -6.66 | 1.25        | 1.33     |
| 11  | A40   | 237  | LEU  | C-N   | -6.66 | 1.23        | 1.33     |
| 10  | C16   | 1630 | LEU  | C-N   | -6.66 | 1.25        | 1.33     |
| 10  | C     | 1310 | HIS  | C-N   | 6.66  | 1.43        | 1.33     |
| 10  | C8    | 1430 | ARG  | C-N   | -6.66 | 1.25        | 1.33     |
| 10  | C24   | 48   | PRO  | N-CD  | -6.66 | 1.38        | 1.47     |
| 11  | A40   | 853  | LEU  | C-N   | -6.66 | 1.25        | 1.33     |
| 10  | C16   | 880  | GLU  | C-N   | 6.66  | 1.43        | 1.33     |
| 18  | B8    | 1098 | MET  | C-N   | -6.66 | 1.25        | 1.33     |
| 10  | C24   | 984  | SER  | C-N   | -6.66 | 1.25        | 1.33     |
| 23  | J16   | 729  | ARG  | C-N   | 6.66  | 1.42        | 1.33     |
| 18  | B     | 1486 | ASP  | C-N   | -6.65 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 251  | GLY  | C-N   | -6.65 | 1.24        | 1.33     |
| 15  | J     | 594  | GLU  | C-N   | -6.65 | 1.24        | 1.33     |
| 11  | A16   | 853  | LEU  | C-N   | -6.65 | 1.25        | 1.33     |
| 9   | K8    | 728  | GLN  | C-N   | 6.65  | 1.42        | 1.33     |
| 10  | C16   | 684  | PRO  | C-N   | -6.65 | 1.25        | 1.33     |
| 9   | K     | 1015 | ILE  | C-N   | -6.65 | 1.24        | 1.33     |
| 10  | C24   | 1753 | THR  | C-N   | -6.65 | 1.24        | 1.33     |
| 18  | B8    | 1486 | ASP  | C-N   | -6.65 | 1.24        | 1.33     |
| 10  | C32   | 880  | GLU  | C-N   | 6.65  | 1.43        | 1.33     |
| 18  | B     | 1217 | GLU  | C-N   | -6.64 | 1.24        | 1.33     |
| 19  | 4     | 375  | ASP  | C-N   | -6.64 | 1.25        | 1.34     |
| 5   | P16   | 541  | ARG  | C-N   | -6.64 | 1.24        | 1.33     |
| 18  | B8    | 1217 | GLU  | C-N   | -6.64 | 1.24        | 1.33     |
| 7   | Q     | 172  | LYS  | C-N   | -6.64 | 1.25        | 1.33     |
| 7   | Q8    | 190  | PRO  | N-CD  | 6.64  | 1.57        | 1.47     |
| 11  | A32   | 237  | LEU  | C-N   | -6.64 | 1.23        | 1.33     |
| 18  | B     | 281  | MET  | C-N   | -6.64 | 1.25        | 1.33     |
| 18  | B     | 1070 | GLY  | C-N   | 6.64  | 1.42        | 1.33     |
| 18  | B8    | 1639 | ALA  | C-N   | -6.64 | 1.25        | 1.34     |
| 20  | E     | 278  | GLU  | C-N   | -6.64 | 1.25        | 1.33     |
| 10  | C24   | 1630 | LEU  | C-N   | -6.64 | 1.25        | 1.33     |
| 22  | I24   | 158  | SER  | C-N   | -6.64 | 1.25        | 1.33     |
| 10  | C24   | 283  | SER  | C-N   | -6.63 | 1.24        | 1.33     |
| 10  | C8    | 880  | GLU  | C-N   | 6.63  | 1.43        | 1.33     |
| 21  | H8    | 340  | GLU  | C-N   | -6.63 | 1.25        | 1.33     |
| 22  | I     | 158  | SER  | C-N   | -6.63 | 1.25        | 1.33     |
| 5   | P     | 541  | ARG  | C-N   | -6.63 | 1.25        | 1.33     |
| 7   | Q8    | 57   | ASN  | C-N   | -6.63 | 1.25        | 1.33     |
| 10  | C8    | 1135 | TYR  | C-N   | -6.63 | 1.23        | 1.33     |
| 11  | A16   | 290  | LYS  | C-N   | -6.63 | 1.25        | 1.33     |
| 7   | Q     | 190  | PRO  | N-CD  | 6.63  | 1.57        | 1.47     |
| 10  | C8    | 1189 | LYS  | C-N   | -6.63 | 1.25        | 1.33     |
| 9   | K8    | 660  | GLN  | C-N   | -6.63 | 1.25        | 1.33     |
| 14  | W     | 687  | ARG  | C-N   | -6.63 | 1.25        | 1.33     |
| 19  | 4     | 34   | TYR  | C-N   | -6.63 | 1.25        | 1.33     |
| 9   | K     | 1131 | GLU  | C-N   | -6.63 | 1.25        | 1.33     |
| 10  | C24   | 426  | LEU  | C-N   | -6.63 | 1.25        | 1.33     |
| 10  | C     | 251  | GLY  | C-N   | -6.63 | 1.24        | 1.33     |
| 11  | A32   | 853  | LEU  | C-N   | -6.63 | 1.25        | 1.33     |
| 10  | C     | 283  | SER  | C-N   | -6.62 | 1.24        | 1.33     |
| 18  | B     | 1639 | ALA  | C-N   | -6.62 | 1.25        | 1.34     |
| 9   | K     | 914  | GLN  | C-N   | -6.62 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C16   | 1135 | TYR  | C-N   | -6.62 | 1.23        | 1.33     |
| 3   | N16   | 1    | MET  | C-N   | -6.62 | 1.26        | 1.33     |
| 10  | C16   | 48   | PRO  | N-CD  | -6.62 | 1.38        | 1.47     |
| 19  | 48    | 146  | ASN  | C-N   | -6.62 | 1.25        | 1.33     |
| 9   | K     | 1050 | GLU  | C-N   | 6.62  | 1.43        | 1.33     |
| 2   | M8    | 639  | GLN  | C-N   | 6.62  | 1.43        | 1.33     |
| 6   | O8    | 133  | LEU  | C-N   | -6.62 | 1.24        | 1.33     |
| 15  | J     | 540  | GLY  | C-N   | 6.62  | 1.42        | 1.33     |
| 18  | B8    | 1475 | SER  | C-N   | 6.62  | 1.43        | 1.33     |
| 3   | N     | 1    | MET  | C-N   | -6.62 | 1.26        | 1.33     |
| 3   | N     | 281  | ASN  | C-N   | 6.62  | 1.42        | 1.33     |
| 10  | C32   | 48   | PRO  | N-CD  | -6.62 | 1.38        | 1.47     |
| 2   | M8    | 832  | PRO  | N-CD  | -6.61 | 1.38        | 1.47     |
| 3   | N8    | 116  | ILE  | C-N   | -6.61 | 1.23        | 1.33     |
| 9   | K     | 1231 | PRO  | N-CD  | -6.61 | 1.38        | 1.47     |
| 14  | W     | 662  | GLU  | C-N   | -6.61 | 1.25        | 1.33     |
| 10  | C8    | 1002 | LEU  | C-N   | 6.61  | 1.42        | 1.33     |
| 19  | 48    | 212  | ASP  | C-N   | -6.61 | 1.24        | 1.33     |
| 23  | J24   | 593  | VAL  | C-N   | -6.61 | 1.25        | 1.33     |
| 10  | C8    | 283  | SER  | C-N   | -6.61 | 1.24        | 1.33     |
| 11  | A32   | 309  | VAL  | C-N   | -6.61 | 1.26        | 1.33     |
| 1   | R8    | 1149 | HIS  | C-N   | -6.61 | 1.25        | 1.33     |
| 9   | K     | 881  | GLY  | C-N   | -6.61 | 1.25        | 1.33     |
| 2   | M16   | 254  | LEU  | C-N   | 6.61  | 1.42        | 1.33     |
| 11  | A40   | 800  | SER  | C-N   | -6.61 | 1.24        | 1.33     |
| 1   | R     | 1246 | LYS  | C-N   | 6.60  | 1.41        | 1.33     |
| 10  | C24   | 1135 | TYR  | C-N   | -6.60 | 1.23        | 1.33     |
| 19  | 48    | 246  | ALA  | C-N   | 6.60  | 1.40        | 1.33     |
| 15  | J     | 625  | GLU  | C-N   | -6.60 | 1.25        | 1.33     |
| 10  | C8    | 684  | PRO  | C-N   | -6.60 | 1.25        | 1.33     |
| 11  | A32   | 290  | LYS  | C-N   | -6.60 | 1.25        | 1.33     |
| 19  | 4     | 146  | ASN  | C-N   | -6.60 | 1.25        | 1.33     |
| 10  | C32   | 988  | GLN  | C-N   | -6.60 | 1.25        | 1.33     |
| 18  | B8    | 1831 | LEU  | C-N   | -6.60 | 1.25        | 1.33     |
| 5   | P     | 696  | ALA  | C-N   | -6.60 | 1.25        | 1.33     |
| 9   | K8    | 814  | ASN  | C-N   | -6.60 | 1.24        | 1.34     |
| 9   | K8    | 914  | GLN  | C-N   | -6.60 | 1.25        | 1.34     |
| 17  | F24   | 75   | ALA  | C-N   | -6.60 | 1.25        | 1.33     |
| 2   | M     | 832  | PRO  | N-CD  | -6.59 | 1.38        | 1.47     |
| 6   | O16   | 133  | LEU  | C-N   | -6.59 | 1.24        | 1.33     |
| 10  | C24   | 1023 | LEU  | C-N   | -6.59 | 1.25        | 1.33     |
| 13  | V     | 816  | LYS  | C-N   | 6.59  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 20  | E8    | 278  | GLU  | C-N   | -6.59 | 1.25        | 1.33     |
| 22  | I16   | 143  | LEU  | C-N   | 6.59  | 1.44        | 1.33     |
| 2   | M16   | 771  | ASN  | C-N   | -6.59 | 1.25        | 1.33     |
| 5   | P8    | 570  | GLY  | C-N   | 6.59  | 1.43        | 1.33     |
| 5   | P16   | 648  | LEU  | C-N   | -6.59 | 1.25        | 1.33     |
| 10  | C     | 1189 | LYS  | C-N   | -6.59 | 1.25        | 1.33     |
| 19  | 4     | 212  | ASP  | C-N   | -6.59 | 1.24        | 1.33     |
| 12  | A48   | 853  | LEU  | C-N   | -6.59 | 1.25        | 1.33     |
| 3   | N16   | 116  | ILE  | C-N   | -6.59 | 1.23        | 1.33     |
| 5   | P8    | 534  | VAL  | C-N   | -6.59 | 1.25        | 1.33     |
| 21  | H     | 368  | ALA  | C-N   | -6.59 | 1.24        | 1.34     |
| 10  | C32   | 984  | SER  | C-N   | -6.59 | 1.25        | 1.33     |
| 12  | A     | 309  | VAL  | C-N   | -6.59 | 1.26        | 1.33     |
| 5   | P     | 534  | VAL  | C-N   | -6.59 | 1.25        | 1.33     |
| 5   | P     | 570  | GLY  | C-N   | 6.59  | 1.43        | 1.33     |
| 10  | C     | 880  | GLU  | C-N   | 6.59  | 1.42        | 1.33     |
| 18  | B     | 1266 | LEU  | C-N   | -6.59 | 1.25        | 1.33     |
| 21  | H8    | 368  | ALA  | C-N   | -6.59 | 1.24        | 1.34     |
| 5   | P16   | 570  | GLY  | C-N   | 6.58  | 1.43        | 1.33     |
| 2   | M8    | 771  | ASN  | C-N   | -6.58 | 1.25        | 1.33     |
| 12  | A     | 290  | LYS  | C-N   | -6.58 | 1.25        | 1.33     |
| 1   | R     | 1149 | HIS  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | M     | 771  | ASN  | C-N   | -6.58 | 1.25        | 1.33     |
| 9   | K     | 814  | ASN  | C-N   | -6.58 | 1.24        | 1.34     |
| 18  | B     | 1911 | LEU  | C-N   | -6.58 | 1.25        | 1.33     |
| 18  | B8    | 103  | ILE  | C-N   | -6.58 | 1.25        | 1.33     |
| 3   | N     | 116  | ILE  | C-N   | -6.58 | 1.23        | 1.33     |
| 11  | A40   | 309  | VAL  | C-N   | -6.58 | 1.26        | 1.33     |
| 11  | A32   | 800  | SER  | C-N   | -6.58 | 1.24        | 1.33     |
| 12  | A48   | 800  | SER  | C-N   | -6.58 | 1.24        | 1.33     |
| 2   | M16   | 639  | GLN  | C-N   | 6.58  | 1.43        | 1.33     |
| 9   | K8    | 1131 | GLU  | C-N   | -6.58 | 1.25        | 1.33     |
| 10  | C24   | 684  | PRO  | C-N   | -6.58 | 1.25        | 1.33     |
| 9   | K     | 905  | ASP  | C-N   | -6.58 | 1.25        | 1.33     |
| 9   | K8    | 1050 | GLU  | C-N   | 6.58  | 1.42        | 1.33     |
| 13  | V     | 789  | GLU  | C-N   | -6.58 | 1.24        | 1.34     |
| 18  | B     | 1831 | LEU  | C-N   | -6.58 | 1.25        | 1.33     |
| 22  | I8    | 158  | SER  | C-N   | -6.58 | 1.25        | 1.33     |
| 2   | M16   | 832  | PRO  | N-CD  | -6.57 | 1.38        | 1.47     |
| 18  | B     | 103  | ILE  | C-N   | -6.57 | 1.25        | 1.33     |
| 18  | B8    | 1070 | GLY  | C-N   | 6.57  | 1.42        | 1.33     |
| 5   | P16   | 534  | VAL  | C-N   | -6.57 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 1042 | HIS  | C-N   | -6.57 | 1.25        | 1.33     |
| 6   | O     | 133  | LEU  | C-N   | -6.57 | 1.24        | 1.33     |
| 9   | K     | 1088 | ASP  | C-N   | 6.57  | 1.42        | 1.33     |
| 10  | C16   | 426  | LEU  | C-N   | -6.57 | 1.25        | 1.33     |
| 10  | C16   | 1430 | ARG  | C-N   | -6.57 | 1.25        | 1.33     |
| 10  | C     | 1135 | TYR  | C-N   | -6.57 | 1.23        | 1.33     |
| 19  | 4     | 129  | GLU  | C-N   | -6.57 | 1.24        | 1.33     |
| 22  | I16   | 158  | SER  | C-N   | -6.57 | 1.25        | 1.33     |
| 10  | C32   | 426  | LEU  | C-N   | -6.57 | 1.25        | 1.33     |
| 1   | R16   | 1246 | LYS  | C-N   | 6.57  | 1.41        | 1.33     |
| 5   | P8    | 648  | LEU  | C-N   | -6.57 | 1.25        | 1.33     |
| 17  | F     | 75   | ALA  | C-N   | -6.57 | 1.25        | 1.33     |
| 18  | B8    | 1561 | LEU  | C-N   | -6.57 | 1.25        | 1.33     |
| 21  | H16   | 340  | GLU  | C-N   | -6.57 | 1.25        | 1.33     |
| 10  | C32   | 684  | PRO  | C-N   | -6.57 | 1.25        | 1.33     |
| 2   | M     | 639  | GLN  | C-N   | 6.56  | 1.43        | 1.33     |
| 11  | A32   | 464  | GLY  | C-N   | -6.56 | 1.24        | 1.33     |
| 1   | R     | 1135 | SER  | C-N   | -6.56 | 1.25        | 1.33     |
| 1   | R8    | 1246 | LYS  | C-N   | 6.56  | 1.41        | 1.33     |
| 2   | M8    | 463  | LEU  | C-N   | 6.56  | 1.43        | 1.33     |
| 11  | A16   | 800  | SER  | C-N   | -6.56 | 1.24        | 1.33     |
| 2   | M16   | 463  | LEU  | C-N   | 6.56  | 1.43        | 1.33     |
| 9   | K8    | 682  | LYS  | C-N   | -6.56 | 1.25        | 1.33     |
| 9   | K8    | 1231 | PRO  | N-CD  | -6.56 | 1.38        | 1.47     |
| 12  | A     | 800  | SER  | C-N   | -6.56 | 1.24        | 1.33     |
| 21  | H24   | 368  | ALA  | C-N   | -6.56 | 1.25        | 1.34     |
| 1   | R8    | 1135 | SER  | C-N   | -6.56 | 1.25        | 1.33     |
| 17  | F8    | 75   | ALA  | C-N   | -6.55 | 1.25        | 1.33     |
| 18  | B8    | 1266 | LEU  | C-N   | -6.55 | 1.25        | 1.33     |
| 19  | 48    | 87   | GLN  | C-N   | -6.55 | 1.25        | 1.33     |
| 10  | C32   | 1135 | TYR  | C-N   | -6.55 | 1.23        | 1.33     |
| 19  | 4     | 246  | ALA  | C-N   | 6.55  | 1.40        | 1.33     |
| 5   | P     | 648  | LEU  | C-N   | -6.55 | 1.25        | 1.33     |
| 6   | O16   | 241  | PRO  | N-CD  | 6.55  | 1.56        | 1.47     |
| 17  | F16   | 75   | ALA  | C-N   | -6.55 | 1.25        | 1.33     |
| 19  | 4     | 251  | ARG  | C-N   | -6.55 | 1.24        | 1.33     |
| 10  | C24   | 988  | GLN  | C-N   | -6.55 | 1.25        | 1.33     |
| 10  | C24   | 1430 | ARG  | C-N   | -6.55 | 1.25        | 1.33     |
| 10  | C     | 684  | PRO  | C-N   | -6.55 | 1.25        | 1.33     |
| 18  | B     | 1882 | ASN  | C-N   | 6.55  | 1.43        | 1.33     |
| 1   | R8    | 1376 | LYS  | C-N   | 6.54  | 1.42        | 1.33     |
| 10  | C16   | 988  | GLN  | C-N   | -6.54 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M     | 339  | GLU  | C-N   | 6.54  | 1.42        | 1.33     |
| 6   | O8    | 241  | PRO  | N-CD  | 6.54  | 1.56        | 1.47     |
| 10  | C     | 48   | PRO  | N-CD  | -6.54 | 1.38        | 1.47     |
| 6   | O     | 241  | PRO  | N-CD  | 6.54  | 1.56        | 1.47     |
| 10  | C16   | 1023 | LEU  | C-N   | -6.54 | 1.25        | 1.33     |
| 11  | A40   | 290  | LYS  | C-N   | -6.54 | 1.25        | 1.33     |
| 10  | C32   | 283  | SER  | C-N   | -6.54 | 1.24        | 1.33     |
| 2   | M     | 463  | LEU  | C-N   | 6.54  | 1.43        | 1.33     |
| 9   | K     | 728  | GLN  | C-N   | 6.54  | 1.42        | 1.33     |
| 10  | C     | 426  | LEU  | C-N   | -6.54 | 1.25        | 1.33     |
| 11  | A32   | 2    | ALA  | C-N   | 6.54  | 1.43        | 1.33     |
| 9   | K     | 682  | LYS  | C-N   | -6.54 | 1.25        | 1.33     |
| 13  | V     | 876  | PRO  | C-N   | -6.54 | 1.24        | 1.33     |
| 10  | C32   | 1002 | LEU  | C-N   | 6.54  | 1.41        | 1.33     |
| 10  | C     | 1002 | LEU  | C-N   | 6.53  | 1.41        | 1.33     |
| 19  | 4     | 87   | GLN  | C-N   | -6.53 | 1.25        | 1.33     |
| 21  | H     | 340  | GLU  | C-N   | -6.53 | 1.25        | 1.33     |
| 23  | J24   | 729  | ARG  | C-N   | 6.53  | 1.42        | 1.33     |
| 10  | C32   | 49   | PRO  | N-CD  | -6.53 | 1.38        | 1.47     |
| 23  | J32   | 595  | THR  | C-N   | -6.53 | 1.25        | 1.33     |
| 1   | R16   | 1187 | ARG  | C-N   | -6.53 | 1.22        | 1.33     |
| 18  | B     | 1346 | ILE  | C-N   | -6.53 | 1.25        | 1.33     |
| 21  | H24   | 340  | GLU  | C-N   | -6.53 | 1.25        | 1.33     |
| 9   | K     | 1097 | VAL  | C-N   | 6.53  | 1.42        | 1.34     |
| 1   | R     | 1376 | LYS  | C-N   | 6.53  | 1.42        | 1.33     |
| 18  | B8    | 1481 | MET  | C-N   | 6.53  | 1.42        | 1.34     |
| 5   | P8    | 696  | ALA  | C-N   | -6.52 | 1.25        | 1.33     |
| 10  | C16   | 283  | SER  | C-N   | -6.52 | 1.24        | 1.33     |
| 11  | A24   | 800  | SER  | C-N   | -6.52 | 1.24        | 1.33     |
| 15  | J     | 553  | GLU  | C-N   | -6.52 | 1.25        | 1.33     |
| 11  | A40   | 2    | ALA  | C-N   | 6.52  | 1.43        | 1.33     |
| 18  | B8    | 1882 | ASN  | C-N   | 6.52  | 1.43        | 1.33     |
| 11  | A24   | 290  | LYS  | C-N   | -6.52 | 1.25        | 1.33     |
| 12  | A48   | 464  | GLY  | C-N   | -6.52 | 1.24        | 1.33     |
| 1   | R16   | 1241 | TYR  | C-N   | 6.51  | 1.42        | 1.33     |
| 12  | A     | 612  | GLN  | C-N   | -6.51 | 1.25        | 1.33     |
| 10  | C8    | 48   | PRO  | N-CD  | -6.51 | 1.38        | 1.47     |
| 19  | 48    | 251  | ARG  | C-N   | -6.51 | 1.24        | 1.33     |
| 23  | J8    | 729  | ARG  | C-N   | 6.51  | 1.42        | 1.33     |
| 2   | M16   | 339  | GLU  | C-N   | 6.51  | 1.42        | 1.33     |
| 23  | J24   | 595  | THR  | C-N   | -6.51 | 1.25        | 1.33     |
| 2   | M16   | 379  | GLN  | C-N   | -6.51 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K8    | 1088 | ASP  | C-N   | 6.51  | 1.42        | 1.33     |
| 19  | 48    | 129  | GLU  | C-N   | -6.51 | 1.24        | 1.33     |
| 2   | M8    | 339  | GLU  | C-N   | 6.51  | 1.42        | 1.33     |
| 18  | B     | 1481 | MET  | C-N   | 6.51  | 1.42        | 1.34     |
| 9   | K     | 973  | ASN  | C-N   | -6.51 | 1.25        | 1.34     |
| 12  | A     | 464  | GLY  | C-N   | -6.51 | 1.24        | 1.33     |
| 14  | W     | 679  | LYS  | C-N   | -6.51 | 1.25        | 1.33     |
| 21  | H16   | 368  | ALA  | C-N   | -6.51 | 1.25        | 1.34     |
| 11  | A24   | 2    | ALA  | C-N   | 6.51  | 1.43        | 1.33     |
| 10  | C32   | 511  | PRO  | N-CD  | -6.51 | 1.38        | 1.47     |
| 11  | A16   | 464  | GLY  | C-N   | -6.50 | 1.24        | 1.33     |
| 14  | W     | 786  | LEU  | C-N   | -6.50 | 1.25        | 1.33     |
| 11  | A16   | 612  | GLN  | C-N   | -6.50 | 1.25        | 1.33     |
| 18  | B8    | 687  | SER  | C-N   | 6.50  | 1.43        | 1.33     |
| 20  | E8    | 331  | GLY  | C-N   | -6.50 | 1.25        | 1.33     |
| 18  | B8    | 1792 | SER  | C-N   | 6.50  | 1.42        | 1.33     |
| 5   | P8    | 121  | LEU  | C-N   | -6.50 | 1.25        | 1.33     |
| 23  | J16   | 593  | VAL  | C-N   | -6.50 | 1.25        | 1.33     |
| 5   | P16   | 696  | ALA  | C-N   | -6.50 | 1.25        | 1.33     |
| 10  | C     | 511  | PRO  | N-CD  | -6.50 | 1.38        | 1.47     |
| 1   | R8    | 1241 | TYR  | C-N   | 6.50  | 1.42        | 1.33     |
| 2   | M8    | 379  | GLN  | C-N   | -6.50 | 1.25        | 1.33     |
| 1   | R16   | 1376 | LYS  | C-N   | 6.50  | 1.42        | 1.33     |
| 2   | M8    | 341  | ASP  | C-N   | 6.49  | 1.42        | 1.33     |
| 10  | C8    | 988  | GLN  | C-N   | -6.49 | 1.25        | 1.33     |
| 12  | A48   | 612  | GLN  | C-N   | -6.49 | 1.25        | 1.33     |
| 23  | J8    | 593  | VAL  | C-N   | -6.49 | 1.25        | 1.33     |
| 5   | P     | 250  | VAL  | C-N   | -6.49 | 1.25        | 1.33     |
| 9   | K8    | 973  | ASN  | C-N   | -6.49 | 1.25        | 1.34     |
| 1   | R16   | 1149 | HIS  | C-N   | -6.49 | 1.25        | 1.33     |
| 10  | C24   | 1002 | LEU  | C-N   | 6.49  | 1.41        | 1.33     |
| 15  | J     | 602  | GLN  | C-N   | -6.49 | 1.25        | 1.33     |
| 18  | B8    | 1827 | ALA  | C-N   | -6.49 | 1.25        | 1.33     |
| 2   | M16   | 157  | GLY  | C-N   | 6.49  | 1.42        | 1.33     |
| 18  | B     | 265  | CYS  | C-N   | -6.49 | 1.25        | 1.33     |
| 23  | J32   | 729  | ARG  | C-N   | 6.49  | 1.42        | 1.33     |
| 12  | A48   | 808  | CYS  | C-N   | -6.49 | 1.26        | 1.33     |
| 9   | K8    | 905  | ASP  | C-N   | -6.48 | 1.25        | 1.33     |
| 12  | A     | 808  | CYS  | C-N   | -6.48 | 1.26        | 1.33     |
| 5   | P16   | 121  | LEU  | C-N   | -6.48 | 1.25        | 1.33     |
| 10  | C24   | 49   | PRO  | N-CD  | -6.48 | 1.38        | 1.47     |
| 18  | B8    | 382  | ASP  | C-N   | 6.48  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | R16   | 1135 | SER  | C-N   | -6.48 | 1.25        | 1.33     |
| 11  | A24   | 612  | GLN  | C-N   | -6.48 | 1.25        | 1.33     |
| 10  | C     | 988  | GLN  | C-N   | -6.48 | 1.25        | 1.33     |
| 18  | B8    | 265  | CYS  | C-N   | -6.48 | 1.25        | 1.33     |
| 2   | M     | 379  | GLN  | C-N   | -6.48 | 1.25        | 1.33     |
| 11  | A40   | 3    | ASN  | C-N   | 6.48  | 1.43        | 1.33     |
| 11  | A40   | 464  | GLY  | C-N   | -6.48 | 1.24        | 1.33     |
| 20  | E     | 96   | ARG  | C-N   | -6.48 | 1.25        | 1.34     |
| 5   | P     | 366  | HIS  | C-N   | -6.48 | 1.25        | 1.34     |
| 5   | P8    | 366  | HIS  | C-N   | -6.48 | 1.25        | 1.34     |
| 10  | C24   | 511  | PRO  | N-CD  | -6.48 | 1.38        | 1.47     |
| 1   | R     | 1241 | TYR  | C-N   | 6.47  | 1.42        | 1.33     |
| 5   | P8    | 250  | VAL  | C-N   | -6.47 | 1.25        | 1.33     |
| 10  | C8    | 1480 | PHE  | C-N   | 6.47  | 1.42        | 1.33     |
| 20  | E     | 217  | GLN  | C-N   | -6.47 | 1.25        | 1.33     |
| 9   | K     | 679  | LEU  | C-N   | -6.47 | 1.25        | 1.34     |
| 18  | B     | 382  | ASP  | C-N   | 6.47  | 1.42        | 1.33     |
| 18  | B8    | 1755 | ALA  | C-N   | -6.47 | 1.25        | 1.33     |
| 10  | C24   | 186  | LEU  | C-N   | -6.47 | 1.24        | 1.33     |
| 10  | C     | 186  | LEU  | C-N   | -6.47 | 1.24        | 1.33     |
| 1   | R     | 1187 | ARG  | C-N   | -6.47 | 1.23        | 1.33     |
| 10  | C32   | 1480 | PHE  | C-N   | 6.47  | 1.42        | 1.33     |
| 13  | V     | 802  | ILE  | C-N   | -6.46 | 1.25        | 1.33     |
| 10  | C     | 1023 | LEU  | C-N   | -6.46 | 1.25        | 1.33     |
| 20  | E8    | 96   | ARG  | C-N   | -6.46 | 1.25        | 1.34     |
| 11  | A16   | 2    | ALA  | C-N   | 6.46  | 1.43        | 1.33     |
| 20  | E8    | 131  | PRO  | N-CD  | -6.46 | 1.38        | 1.47     |
| 9   | K8    | 634  | LEU  | C-N   | 6.46  | 1.42        | 1.33     |
| 9   | K8    | 1042 | HIS  | C-N   | -6.46 | 1.25        | 1.33     |
| 10  | C8    | 186  | LEU  | C-N   | -6.46 | 1.24        | 1.33     |
| 11  | A32   | 612  | GLN  | C-N   | -6.46 | 1.25        | 1.33     |
| 10  | C32   | 1430 | ARG  | C-N   | -6.46 | 1.25        | 1.33     |
| 11  | A24   | 3    | ASN  | C-N   | 6.46  | 1.43        | 1.33     |
| 3   | N8    | 1    | MET  | C-N   | -6.46 | 1.26        | 1.33     |
| 5   | P16   | 250  | VAL  | C-N   | -6.46 | 1.25        | 1.33     |
| 18  | B     | 1561 | LEU  | C-N   | -6.46 | 1.25        | 1.33     |
| 2   | M16   | 810  | LEU  | C-N   | 6.46  | 1.42        | 1.33     |
| 10  | C16   | 1002 | LEU  | C-N   | 6.46  | 1.41        | 1.33     |
| 11  | A24   | 464  | GLY  | C-N   | -6.46 | 1.24        | 1.33     |
| 21  | H8    | 372  | GLU  | C-N   | -6.46 | 1.25        | 1.33     |
| 2   | M     | 341  | ASP  | C-N   | 6.45  | 1.42        | 1.33     |
| 10  | C16   | 49   | PRO  | N-CD  | -6.45 | 1.38        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 281  | MET  | C-N   | -6.45 | 1.25        | 1.33     |
| 9   | K     | 634  | LEU  | C-N   | 6.45  | 1.41        | 1.33     |
| 12  | A     | 134  | LYS  | C-N   | 6.45  | 1.42        | 1.33     |
| 18  | B     | 1755 | ALA  | C-N   | -6.45 | 1.25        | 1.33     |
| 12  | A     | 301  | THR  | C-N   | -6.45 | 1.25        | 1.34     |
| 18  | B     | 1827 | ALA  | C-N   | -6.45 | 1.25        | 1.33     |
| 18  | B8    | 1346 | ILE  | C-N   | -6.45 | 1.25        | 1.33     |
| 20  | E     | 331  | GLY  | C-N   | -6.45 | 1.25        | 1.33     |
| 1   | R8    | 1187 | ARG  | C-N   | -6.45 | 1.23        | 1.33     |
| 10  | C8    | 426  | LEU  | C-N   | -6.45 | 1.25        | 1.33     |
| 18  | B     | 1607 | GLY  | C-N   | 6.45  | 1.42        | 1.34     |
| 20  | E     | 131  | PRO  | N-CD  | -6.45 | 1.38        | 1.47     |
| 10  | C16   | 1480 | PHE  | C-N   | 6.44  | 1.42        | 1.33     |
| 18  | B     | 687  | SER  | C-N   | 6.44  | 1.43        | 1.33     |
| 9   | K8    | 679  | LEU  | C-N   | -6.44 | 1.25        | 1.34     |
| 10  | C24   | 622  | VAL  | C-N   | -6.44 | 1.24        | 1.33     |
| 11  | A40   | 269  | GLY  | C-N   | -6.44 | 1.24        | 1.33     |
| 18  | B8    | 1013 | VAL  | C-N   | 6.44  | 1.43        | 1.33     |
| 23  | J16   | 595  | THR  | C-N   | -6.44 | 1.25        | 1.33     |
| 10  | C32   | 1023 | LEU  | C-N   | -6.44 | 1.25        | 1.33     |
| 10  | C16   | 511  | PRO  | N-CD  | -6.44 | 1.38        | 1.47     |
| 10  | C32   | 186  | LEU  | C-N   | -6.44 | 1.24        | 1.33     |
| 6   | O8    | 191  | PHE  | C-N   | -6.44 | 1.25        | 1.33     |
| 18  | B     | 1042 | GLU  | C-N   | 6.44  | 1.42        | 1.34     |
| 18  | B     | 1281 | LYS  | C-N   | 6.44  | 1.42        | 1.33     |
| 10  | C24   | 1480 | PHE  | C-N   | 6.44  | 1.42        | 1.33     |
| 10  | C16   | 186  | LEU  | C-N   | -6.43 | 1.24        | 1.33     |
| 10  | C24   | 54   | ARG  | C-N   | 6.43  | 1.42        | 1.34     |
| 14  | W     | 625  | LYS  | C-N   | -6.43 | 1.25        | 1.33     |
| 10  | C8    | 850  | ARG  | C-N   | 6.43  | 1.42        | 1.33     |
| 18  | B8    | 1281 | LYS  | C-N   | 6.43  | 1.42        | 1.33     |
| 10  | C8    | 1023 | LEU  | C-N   | -6.43 | 1.25        | 1.33     |
| 10  | C8    | 511  | PRO  | N-CD  | -6.43 | 1.38        | 1.47     |
| 14  | W     | 655  | ASP  | C-N   | -6.43 | 1.25        | 1.33     |
| 10  | C     | 1480 | PHE  | C-N   | 6.43  | 1.42        | 1.33     |
| 11  | A16   | 269  | GLY  | C-N   | -6.43 | 1.24        | 1.33     |
| 15  | J     | 693  | VAL  | C-N   | -6.43 | 1.25        | 1.33     |
| 10  | C16   | 886  | GLU  | C-N   | 6.43  | 1.42        | 1.33     |
| 15  | J     | 581  | VAL  | C-N   | -6.43 | 1.25        | 1.33     |
| 10  | C8    | 855  | VAL  | C-N   | 6.43  | 1.42        | 1.33     |
| 10  | C32   | 855  | VAL  | C-N   | 6.43  | 1.42        | 1.33     |
| 9   | K8    | 1120 | GLY  | C-N   | 6.42  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A16   | 3    | ASN  | C-N   | 6.42  | 1.43        | 1.33     |
| 11  | A32   | 3    | ASN  | C-N   | 6.42  | 1.43        | 1.33     |
| 18  | B8    | 1607 | GLY  | C-N   | 6.42  | 1.42        | 1.34     |
| 12  | A48   | 301  | THR  | C-N   | -6.42 | 1.25        | 1.34     |
| 10  | C     | 855  | VAL  | C-N   | 6.42  | 1.42        | 1.33     |
| 10  | C     | 622  | VAL  | C-N   | -6.42 | 1.25        | 1.33     |
| 21  | H     | 372  | GLU  | C-N   | -6.42 | 1.25        | 1.33     |
| 11  | A40   | 859  | ARG  | C-N   | -6.42 | 1.24        | 1.33     |
| 18  | B     | 1792 | SER  | C-N   | 6.42  | 1.42        | 1.33     |
| 10  | C32   | 54   | ARG  | C-N   | 6.42  | 1.42        | 1.34     |
| 12  | A48   | 269  | GLY  | C-N   | -6.42 | 1.24        | 1.33     |
| 1   | R     | 1254 | LEU  | C-N   | -6.42 | 1.25        | 1.33     |
| 2   | M     | 810  | LEU  | C-N   | 6.42  | 1.42        | 1.33     |
| 7   | Q8    | 226  | THR  | C-N   | 6.42  | 1.42        | 1.33     |
| 21  | H8    | 159  | TYR  | C-N   | -6.42 | 1.24        | 1.33     |
| 5   | P16   | 366  | HIS  | C-N   | -6.41 | 1.25        | 1.34     |
| 9   | K8    | 1097 | VAL  | C-N   | 6.41  | 1.42        | 1.34     |
| 20  | E     | 5    | PRO  | N-CD  | -6.41 | 1.38        | 1.47     |
| 10  | C32   | 1797 | CYS  | C-N   | 6.41  | 1.43        | 1.33     |
| 19  | 4     | 369  | VAL  | C-N   | -6.41 | 1.24        | 1.33     |
| 1   | R     | 1371 | LEU  | C-N   | 6.41  | 1.42        | 1.33     |
| 13  | V     | 780  | CYS  | C-N   | -6.41 | 1.25        | 1.33     |
| 10  | C32   | 622  | VAL  | C-N   | -6.41 | 1.25        | 1.33     |
| 11  | A32   | 859  | ARG  | C-N   | -6.41 | 1.24        | 1.33     |
| 2   | M8    | 157  | GLY  | C-N   | 6.41  | 1.42        | 1.33     |
| 5   | P     | 121  | LEU  | C-N   | -6.41 | 1.25        | 1.33     |
| 7   | Q16   | 226  | THR  | C-N   | 6.41  | 1.42        | 1.33     |
| 10  | C16   | 54   | ARG  | C-N   | 6.41  | 1.42        | 1.34     |
| 5   | P8    | 576  | GLU  | C-N   | -6.40 | 1.25        | 1.34     |
| 14  | W     | 666  | LYS  | C-N   | -6.40 | 1.26        | 1.33     |
| 11  | A40   | 516  | PRO  | N-CD  | 6.40  | 1.56        | 1.47     |
| 10  | C     | 1664 | SER  | C-N   | 6.40  | 1.42        | 1.33     |
| 1   | R8    | 1371 | LEU  | C-N   | 6.40  | 1.42        | 1.33     |
| 10  | C16   | 855  | VAL  | C-N   | 6.40  | 1.42        | 1.33     |
| 13  | V     | 783  | TRP  | C-N   | -6.40 | 1.25        | 1.33     |
| 10  | C     | 54   | ARG  | C-N   | 6.40  | 1.42        | 1.34     |
| 19  | 48    | 369  | VAL  | C-N   | -6.40 | 1.24        | 1.33     |
| 12  | A     | 511  | SER  | C-N   | -6.40 | 1.25        | 1.33     |
| 6   | O     | 191  | PHE  | C-N   | -6.40 | 1.25        | 1.33     |
| 20  | E8    | 217  | GLN  | C-N   | -6.40 | 1.25        | 1.33     |
| 1   | R8    | 1254 | LEU  | C-N   | -6.39 | 1.25        | 1.33     |
| 5   | P     | 576  | GLU  | C-N   | -6.39 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A48   | 290  | LYS  | C-N   | -6.39 | 1.25        | 1.33     |
| 11  | A40   | 612  | GLN  | C-N   | -6.39 | 1.25        | 1.33     |
| 18  | B     | 1581 | GLY  | C-N   | 6.39  | 1.42        | 1.33     |
| 10  | C8    | 54   | ARG  | C-N   | 6.39  | 1.42        | 1.34     |
| 18  | B     | 300  | VAL  | C-N   | 6.39  | 1.42        | 1.33     |
| 18  | B8    | 1508 | PRO  | N-CD  | -6.39 | 1.38        | 1.47     |
| 12  | A48   | 209  | GLU  | C-N   | -6.39 | 1.25        | 1.33     |
| 3   | N8    | 225  | PRO  | N-CD  | -6.38 | 1.38        | 1.47     |
| 18  | B8    | 300  | VAL  | C-N   | 6.38  | 1.42        | 1.33     |
| 11  | A16   | 301  | THR  | C-N   | -6.38 | 1.25        | 1.34     |
| 23  | J8    | 595  | THR  | C-N   | -6.38 | 1.25        | 1.33     |
| 12  | A48   | 511  | SER  | C-N   | -6.38 | 1.25        | 1.33     |
| 9   | K     | 782  | ILE  | C-N   | -6.38 | 1.24        | 1.33     |
| 19  | 48    | 195  | ARG  | C-N   | 6.38  | 1.42        | 1.33     |
| 9   | K8    | 730  | SER  | C-N   | -6.38 | 1.25        | 1.33     |
| 11  | A24   | 516  | PRO  | N-CD  | 6.38  | 1.56        | 1.47     |
| 11  | A16   | 516  | PRO  | N-CD  | 6.38  | 1.56        | 1.47     |
| 18  | B8    | 1581 | GLY  | C-N   | 6.38  | 1.42        | 1.33     |
| 21  | H16   | 372  | GLU  | C-N   | -6.38 | 1.25        | 1.33     |
| 13  | V     | 874  | GLY  | C-N   | 6.38  | 1.46        | 1.33     |
| 7   | Q     | 226  | THR  | C-N   | 6.37  | 1.42        | 1.33     |
| 10  | C     | 49   | PRO  | N-CD  | -6.37 | 1.38        | 1.47     |
| 10  | C     | 850  | ARG  | C-N   | 6.37  | 1.42        | 1.33     |
| 18  | B     | 1480 | HIS  | C-N   | -6.37 | 1.25        | 1.33     |
| 20  | E     | 8    | GLU  | C-N   | -6.37 | 1.25        | 1.34     |
| 3   | N8    | 139  | GLY  | C-N   | 6.37  | 1.42        | 1.33     |
| 1   | R16   | 1254 | LEU  | C-N   | -6.37 | 1.25        | 1.33     |
| 5   | P16   | 576  | GLU  | C-N   | -6.37 | 1.25        | 1.34     |
| 9   | K     | 1213 | CYS  | C-N   | 6.37  | 1.43        | 1.33     |
| 10  | C16   | 622  | VAL  | C-N   | -6.37 | 1.25        | 1.33     |
| 12  | A     | 209  | GLU  | C-N   | -6.37 | 1.25        | 1.33     |
| 18  | B8    | 1288 | GLY  | C-N   | -6.37 | 1.24        | 1.33     |
| 2   | M     | 157  | GLY  | C-N   | 6.37  | 1.42        | 1.33     |
| 11  | A16   | 511  | SER  | C-N   | -6.37 | 1.25        | 1.33     |
| 11  | A32   | 511  | SER  | C-N   | -6.37 | 1.25        | 1.33     |
| 20  | E8    | 5    | PRO  | N-CD  | -6.37 | 1.38        | 1.47     |
| 21  | H16   | 159  | TYR  | C-N   | -6.37 | 1.24        | 1.33     |
| 10  | C24   | 886  | GLU  | C-N   | 6.37  | 1.42        | 1.33     |
| 20  | E8    | 318  | LEU  | C-N   | -6.37 | 1.24        | 1.34     |
| 7   | Q8    | 291  | SER  | C-N   | -6.36 | 1.24        | 1.33     |
| 9   | K     | 657  | VAL  | C-N   | -6.36 | 1.25        | 1.33     |
| 10  | C16   | 447  | PHE  | C-N   | 6.36  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1516 | GLN  | C-N   | -6.36 | 1.25        | 1.33     |
| 18  | B     | 1750 | LEU  | C-N   | 6.36  | 1.42        | 1.33     |
| 9   | K     | 730  | SER  | C-N   | -6.36 | 1.25        | 1.33     |
| 12  | A     | 341  | PRO  | C-N   | -6.36 | 1.26        | 1.33     |
| 15  | J     | 688  | PRO  | C-N   | -6.36 | 1.24        | 1.33     |
| 1   | R16   | 1371 | LEU  | C-N   | 6.36  | 1.42        | 1.33     |
| 9   | K8    | 1213 | CYS  | C-N   | 6.36  | 1.43        | 1.33     |
| 10  | C16   | 1797 | CYS  | C-N   | 6.36  | 1.43        | 1.33     |
| 11  | A24   | 859  | ARG  | C-N   | -6.36 | 1.24        | 1.33     |
| 3   | N16   | 88   | GLY  | C-N   | 6.36  | 1.42        | 1.33     |
| 10  | C16   | 1664 | SER  | C-N   | 6.36  | 1.42        | 1.33     |
| 2   | M16   | 341  | ASP  | C-N   | 6.36  | 1.42        | 1.33     |
| 17  | F8    | 73   | GLY  | C-N   | -6.35 | 1.25        | 1.33     |
| 3   | N     | 225  | PRO  | N-CD  | -6.35 | 1.38        | 1.47     |
| 2   | M8    | 810  | LEU  | C-N   | 6.35  | 1.42        | 1.33     |
| 10  | C     | 539  | LEU  | C-N   | -6.35 | 1.25        | 1.33     |
| 11  | A32   | 808  | CYS  | C-N   | -6.35 | 1.26        | 1.33     |
| 11  | A32   | 516  | PRO  | N-CD  | 6.35  | 1.56        | 1.47     |
| 10  | C8    | 1516 | GLN  | C-N   | -6.35 | 1.25        | 1.33     |
| 19  | 48    | 290  | PRO  | N-CD  | 6.35  | 1.56        | 1.47     |
| 10  | C     | 1797 | CYS  | C-N   | 6.35  | 1.43        | 1.33     |
| 21  | H24   | 159  | TYR  | C-N   | -6.35 | 1.24        | 1.33     |
| 21  | H24   | 372  | GLU  | C-N   | -6.35 | 1.25        | 1.33     |
| 3   | N8    | 88   | GLY  | C-N   | 6.34  | 1.42        | 1.33     |
| 10  | C8    | 49   | PRO  | N-CD  | -6.34 | 1.38        | 1.47     |
| 10  | C8    | 1619 | PRO  | C-N   | -6.34 | 1.25        | 1.33     |
| 17  | F16   | 73   | GLY  | C-N   | -6.34 | 1.25        | 1.33     |
| 18  | B8    | 1750 | LEU  | C-N   | 6.34  | 1.42        | 1.33     |
| 3   | N     | 139  | GLY  | C-N   | 6.34  | 1.42        | 1.33     |
| 7   | Q     | 291  | SER  | C-N   | -6.34 | 1.24        | 1.33     |
| 11  | A40   | 301  | THR  | C-N   | -6.34 | 1.25        | 1.34     |
| 10  | C     | 616  | GLN  | C-N   | -6.34 | 1.25        | 1.33     |
| 1   | R     | 1440 | PRO  | N-CD  | 6.34  | 1.56        | 1.47     |
| 6   | O16   | 191  | PHE  | C-N   | -6.34 | 1.25        | 1.33     |
| 15  | J     | 710  | ALA  | C-N   | -6.34 | 1.25        | 1.33     |
| 18  | B8    | 1480 | HIS  | C-N   | -6.34 | 1.25        | 1.33     |
| 19  | 4     | 195  | ARG  | C-N   | 6.34  | 1.42        | 1.33     |
| 22  | I24   | 318  | VAL  | C-N   | -6.34 | 1.25        | 1.33     |
| 22  | I16   | 318  | VAL  | C-N   | -6.34 | 1.25        | 1.33     |
| 10  | C24   | 850  | ARG  | C-N   | 6.34  | 1.42        | 1.33     |
| 16  | A8    | 134  | LYS  | C-N   | 6.34  | 1.41        | 1.33     |
| 18  | B     | 447  | PRO  | N-CD  | 6.34  | 1.56        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 19  | 4     | 290  | PRO  | N-CD  | 6.34  | 1.56        | 1.47     |
| 17  | F24   | 73   | GLY  | C-N   | -6.33 | 1.25        | 1.33     |
| 18  | B8    | 762  | LYS  | C-N   | 6.33  | 1.41        | 1.33     |
| 10  | C32   | 850  | ARG  | C-N   | 6.33  | 1.42        | 1.33     |
| 3   | N16   | 225  | PRO  | N-CD  | -6.33 | 1.38        | 1.47     |
| 7   | Q16   | 291  | SER  | C-N   | -6.33 | 1.24        | 1.33     |
| 9   | K     | 1257 | ALA  | C-N   | -6.33 | 1.25        | 1.33     |
| 11  | A16   | 859  | ARG  | C-N   | -6.33 | 1.24        | 1.33     |
| 10  | C16   | 850  | ARG  | C-N   | 6.33  | 1.42        | 1.33     |
| 20  | E     | 318  | LEU  | C-N   | -6.33 | 1.24        | 1.34     |
| 21  | H     | 159  | TYR  | C-N   | -6.33 | 1.24        | 1.33     |
| 9   | K8    | 782  | ILE  | C-N   | -6.32 | 1.24        | 1.33     |
| 11  | A40   | 511  | SER  | C-N   | -6.32 | 1.25        | 1.33     |
| 18  | B     | 1288 | GLY  | C-N   | -6.32 | 1.24        | 1.33     |
| 18  | B     | 849  | SER  | C-N   | 6.32  | 1.43        | 1.33     |
| 18  | B     | 1013 | VAL  | C-N   | 6.32  | 1.43        | 1.33     |
| 18  | B8    | 849  | SER  | C-N   | 6.32  | 1.43        | 1.33     |
| 10  | C32   | 1664 | SER  | C-N   | 6.32  | 1.42        | 1.33     |
| 11  | A40   | 808  | CYS  | C-N   | -6.32 | 1.26        | 1.33     |
| 10  | C32   | 616  | GLN  | C-N   | -6.32 | 1.25        | 1.33     |
| 18  | B     | 1895 | LEU  | C-N   | 6.32  | 1.42        | 1.33     |
| 10  | C32   | 886  | GLU  | C-N   | 6.32  | 1.42        | 1.33     |
| 10  | C32   | 1516 | GLN  | C-N   | -6.32 | 1.25        | 1.33     |
| 10  | C24   | 1619 | PRO  | C-N   | -6.32 | 1.25        | 1.33     |
| 11  | A40   | 341  | PRO  | C-N   | -6.32 | 1.26        | 1.33     |
| 10  | C8    | 616  | GLN  | C-N   | -6.32 | 1.25        | 1.33     |
| 10  | C8    | 886  | GLU  | C-N   | 6.31  | 1.42        | 1.33     |
| 9   | K     | 667  | LEU  | C-N   | -6.31 | 1.25        | 1.33     |
| 9   | K     | 1120 | GLY  | C-N   | 6.31  | 1.42        | 1.34     |
| 18  | B     | 1100 | LEU  | C-N   | -6.31 | 1.25        | 1.33     |
| 12  | A48   | 516  | PRO  | N-CD  | 6.31  | 1.56        | 1.47     |
| 5   | P16   | 322  | CYS  | C-N   | -6.30 | 1.25        | 1.33     |
| 11  | A32   | 301  | THR  | C-N   | -6.30 | 1.25        | 1.34     |
| 5   | P     | 56   | ASN  | C-N   | -6.30 | 1.26        | 1.34     |
| 12  | A     | 516  | PRO  | N-CD  | 6.30  | 1.56        | 1.47     |
| 10  | C24   | 1132 | SER  | C-N   | -6.30 | 1.26        | 1.34     |
| 10  | C32   | 447  | PHE  | C-N   | 6.30  | 1.42        | 1.33     |
| 9   | K     | 1192 | TRP  | C-N   | 6.30  | 1.41        | 1.33     |
| 10  | C24   | 1353 | ASP  | C-N   | 6.30  | 1.42        | 1.33     |
| 12  | A     | 647  | GLY  | C-N   | -6.30 | 1.24        | 1.33     |
| 18  | B     | 1820 | ALA  | C-N   | -6.30 | 1.25        | 1.33     |
| 18  | B8    | 1042 | GLU  | C-N   | 6.29  | 1.41        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | P     | 322  | CYS  | C-N   | -6.29 | 1.25        | 1.33     |
| 10  | C24   | 616  | GLN  | C-N   | -6.29 | 1.25        | 1.33     |
| 11  | A16   | 808  | CYS  | C-N   | -6.29 | 1.26        | 1.33     |
| 17  | F     | 73   | GLY  | C-N   | -6.29 | 1.25        | 1.33     |
| 18  | B     | 1958 | ALA  | C-N   | -6.29 | 1.24        | 1.33     |
| 18  | B8    | 1100 | LEU  | C-N   | -6.29 | 1.25        | 1.33     |
| 1   | R8    | 1440 | PRO  | N-CD  | 6.29  | 1.56        | 1.47     |
| 9   | K     | 1168 | GLU  | C-N   | -6.29 | 1.25        | 1.34     |
| 9   | K8    | 1257 | ALA  | C-N   | -6.29 | 1.25        | 1.33     |
| 18  | B8    | 1884 | LYS  | C-N   | 6.29  | 1.41        | 1.33     |
| 20  | E8    | 8    | GLU  | C-N   | -6.29 | 1.25        | 1.34     |
| 3   | N8    | 208  | LYS  | C-N   | -6.29 | 1.24        | 1.33     |
| 11  | A16   | 341  | PRO  | C-N   | -6.29 | 1.26        | 1.33     |
| 10  | C32   | 1619 | PRO  | C-N   | -6.29 | 1.25        | 1.33     |
| 2   | M8    | 821  | THR  | C-N   | -6.29 | 1.25        | 1.34     |
| 3   | N16   | 139  | GLY  | C-N   | 6.29  | 1.42        | 1.33     |
| 9   | K8    | 667  | LEU  | C-N   | -6.29 | 1.25        | 1.33     |
| 10  | C     | 886  | GLU  | C-N   | 6.29  | 1.42        | 1.33     |
| 11  | A24   | 511  | SER  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C     | 1516 | GLN  | C-N   | -6.28 | 1.25        | 1.33     |
| 9   | K8    | 1168 | GLU  | C-N   | -6.28 | 1.25        | 1.34     |
| 11  | A24   | 301  | THR  | C-N   | -6.28 | 1.25        | 1.34     |
| 14  | W     | 797  | ILE  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C32   | 1132 | SER  | C-N   | -6.28 | 1.26        | 1.34     |
| 5   | P16   | 213  | LYS  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C16   | 616  | GLN  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C     | 1438 | ASN  | C-N   | -6.28 | 1.27        | 1.33     |
| 18  | B     | 233  | ARG  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C16   | 1831 | GLU  | C-N   | -6.28 | 1.25        | 1.33     |
| 10  | C     | 1367 | ALA  | C-N   | 6.28  | 1.42        | 1.33     |
| 1   | R16   | 1440 | PRO  | N-CD  | 6.27  | 1.56        | 1.47     |
| 10  | C16   | 1132 | SER  | C-N   | -6.27 | 1.26        | 1.34     |
| 14  | W     | 619  | ILE  | C-N   | -6.27 | 1.25        | 1.34     |
| 18  | B     | 1508 | PRO  | N-CD  | -6.27 | 1.39        | 1.47     |
| 3   | N     | 88   | GLY  | C-N   | 6.27  | 1.42        | 1.33     |
| 7   | Q8    | 121  | ILE  | C-N   | -6.27 | 1.25        | 1.33     |
| 10  | C24   | 1797 | CYS  | C-N   | 6.27  | 1.42        | 1.33     |
| 20  | E8    | 176  | PRO  | C-N   | -6.27 | 1.25        | 1.33     |
| 10  | C16   | 539  | LEU  | C-N   | -6.27 | 1.25        | 1.33     |
| 12  | A48   | 341  | PRO  | C-N   | -6.27 | 1.26        | 1.33     |
| 9   | K8    | 657  | VAL  | C-N   | -6.27 | 1.25        | 1.33     |
| 1   | R16   | 1148 | LYS  | C-N   | -6.27 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A16   | 209  | GLU  | C-N   | -6.27 | 1.25        | 1.33     |
| 10  | C16   | 1367 | ALA  | C-N   | 6.27  | 1.42        | 1.33     |
| 10  | C8    | 1797 | CYS  | C-N   | 6.27  | 1.42        | 1.33     |
| 18  | B8    | 1820 | ALA  | C-N   | -6.27 | 1.26        | 1.33     |
| 1   | R8    | 1148 | LYS  | C-N   | -6.26 | 1.25        | 1.34     |
| 11  | A24   | 697  | ASN  | C-N   | -6.26 | 1.25        | 1.33     |
| 11  | A32   | 209  | GLU  | C-N   | -6.26 | 1.25        | 1.33     |
| 18  | B     | 1117 | THR  | C-N   | 6.26  | 1.42        | 1.33     |
| 18  | B8    | 1895 | LEU  | C-N   | 6.26  | 1.42        | 1.33     |
| 5   | P8    | 322  | CYS  | C-N   | -6.26 | 1.25        | 1.33     |
| 10  | C     | 1619 | PRO  | C-N   | -6.26 | 1.25        | 1.33     |
| 18  | B     | 762  | LYS  | C-N   | 6.26  | 1.41        | 1.33     |
| 10  | C16   | 1516 | GLN  | C-N   | -6.26 | 1.25        | 1.33     |
| 10  | C16   | 1772 | ASP  | C-N   | 6.26  | 1.42        | 1.33     |
| 22  | I     | 318  | VAL  | C-N   | -6.26 | 1.25        | 1.33     |
| 9   | K8    | 606  | GLU  | C-N   | -6.25 | 1.25        | 1.33     |
| 18  | B8    | 1645 | GLU  | C-N   | -6.25 | 1.25        | 1.33     |
| 3   | N16   | 204  | PRO  | C-N   | 6.25  | 1.41        | 1.33     |
| 9   | K8    | 1192 | TRP  | C-N   | 6.25  | 1.41        | 1.33     |
| 10  | C24   | 1664 | SER  | C-N   | 6.25  | 1.42        | 1.33     |
| 5   | P16   | 56   | ASN  | C-N   | -6.25 | 1.26        | 1.34     |
| 10  | C8    | 1132 | SER  | C-N   | -6.25 | 1.26        | 1.34     |
| 18  | B     | 1884 | LYS  | C-N   | 6.25  | 1.41        | 1.33     |
| 10  | C32   | 539  | LEU  | C-N   | -6.25 | 1.25        | 1.33     |
| 10  | C24   | 539  | LEU  | C-N   | -6.25 | 1.25        | 1.33     |
| 12  | A48   | 859  | ARG  | C-N   | -6.25 | 1.24        | 1.33     |
| 2   | M     | 821  | THR  | C-N   | -6.25 | 1.25        | 1.34     |
| 10  | C24   | 1604 | VAL  | C-N   | 6.25  | 1.42        | 1.33     |
| 18  | B8    | 447  | PRO  | N-CD  | 6.25  | 1.56        | 1.47     |
| 5   | P8    | 56   | ASN  | C-N   | -6.25 | 1.26        | 1.34     |
| 7   | Q16   | 121  | ILE  | C-N   | -6.25 | 1.25        | 1.33     |
| 18  | B     | 829  | GLY  | C-N   | 6.25  | 1.42        | 1.33     |
| 18  | B8    | 829  | GLY  | C-N   | 6.24  | 1.42        | 1.33     |
| 1   | R     | 1148 | LYS  | C-N   | -6.24 | 1.25        | 1.34     |
| 11  | A24   | 209  | GLU  | C-N   | -6.24 | 1.26        | 1.33     |
| 11  | A40   | 36   | ASN  | C-N   | -6.24 | 1.25        | 1.33     |
| 18  | B8    | 639  | ALA  | C-N   | 6.24  | 1.41        | 1.33     |
| 3   | N     | 208  | LYS  | C-N   | -6.24 | 1.25        | 1.33     |
| 1   | R8    | 1389 | GLN  | C-N   | -6.24 | 1.25        | 1.33     |
| 10  | C24   | 447  | PHE  | C-N   | 6.24  | 1.42        | 1.33     |
| 11  | A40   | 209  | GLU  | C-N   | -6.24 | 1.26        | 1.33     |
| 10  | C8    | 1438 | ASN  | C-N   | -6.24 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 154  | LEU  | C-N   | 6.24  | 1.42        | 1.33     |
| 21  | H8    | 255  | LEU  | C-N   | -6.24 | 1.25        | 1.33     |
| 10  | C8    | 923  | PRO  | C-N   | -6.24 | 1.26        | 1.34     |
| 22  | I16   | 282  | GLU  | C-N   | -6.24 | 1.25        | 1.33     |
| 7   | Q16   | 152  | GLY  | C-N   | -6.23 | 1.25        | 1.33     |
| 20  | E8    | 248  | PHE  | C-N   | -6.23 | 1.25        | 1.33     |
| 21  | H     | 255  | LEU  | C-N   | -6.23 | 1.25        | 1.33     |
| 5   | P8    | 64   | ASP  | C-N   | -6.23 | 1.25        | 1.33     |
| 11  | A16   | 144  | LYS  | C-N   | 6.23  | 1.42        | 1.33     |
| 18  | B8    | 1958 | ALA  | C-N   | -6.23 | 1.25        | 1.33     |
| 3   | N16   | 208  | LYS  | C-N   | -6.23 | 1.25        | 1.33     |
| 20  | E     | 481  | LEU  | C-N   | -6.23 | 1.25        | 1.33     |
| 10  | C16   | 1619 | PRO  | C-N   | -6.22 | 1.25        | 1.33     |
| 11  | A24   | 808  | CYS  | C-N   | -6.22 | 1.26        | 1.33     |
| 12  | A48   | 647  | GLY  | C-N   | -6.22 | 1.24        | 1.33     |
| 9   | K     | 642  | ARG  | C-N   | 6.22  | 1.41        | 1.33     |
| 9   | K     | 823  | LEU  | C-N   | -6.22 | 1.24        | 1.33     |
| 11  | A16   | 36   | ASN  | C-N   | -6.22 | 1.25        | 1.33     |
| 11  | A32   | 647  | GLY  | C-N   | -6.22 | 1.24        | 1.33     |
| 12  | A48   | 134  | LYS  | C-N   | 6.22  | 1.41        | 1.33     |
| 9   | K8    | 823  | LEU  | C-N   | -6.22 | 1.24        | 1.33     |
| 10  | C16   | 1353 | ASP  | C-N   | 6.22  | 1.42        | 1.33     |
| 11  | A24   | 36   | ASN  | C-N   | -6.22 | 1.25        | 1.33     |
| 10  | C24   | 316  | ILE  | C-N   | 6.22  | 1.42        | 1.33     |
| 10  | C32   | 1772 | ASP  | C-N   | 6.22  | 1.42        | 1.33     |
| 3   | N8    | 204  | PRO  | C-N   | 6.22  | 1.41        | 1.33     |
| 1   | R16   | 1389 | GLN  | C-N   | -6.22 | 1.25        | 1.33     |
| 22  | I8    | 170  | ALA  | C-N   | -6.22 | 1.25        | 1.33     |
| 10  | C32   | 1438 | ASN  | C-N   | -6.22 | 1.27        | 1.33     |
| 12  | A     | 495  | THR  | C-N   | -6.22 | 1.25        | 1.33     |
| 10  | C     | 1831 | GLU  | C-N   | -6.22 | 1.25        | 1.33     |
| 10  | C8    | 539  | LEU  | C-N   | -6.22 | 1.25        | 1.33     |
| 11  | A24   | 134  | LYS  | C-N   | 6.21  | 1.41        | 1.33     |
| 18  | B8    | 233  | ARG  | C-N   | -6.21 | 1.25        | 1.33     |
| 20  | E     | 176  | PRO  | C-N   | -6.21 | 1.25        | 1.33     |
| 18  | B     | 154  | LEU  | C-N   | 6.21  | 1.42        | 1.33     |
| 10  | C32   | 1831 | GLU  | C-N   | -6.21 | 1.25        | 1.33     |
| 5   | P8    | 213  | LYS  | C-N   | -6.21 | 1.25        | 1.33     |
| 9   | K8    | 1019 | ARG  | C-N   | -6.21 | 1.26        | 1.33     |
| 10  | C16   | 316  | ILE  | C-N   | 6.21  | 1.42        | 1.33     |
| 10  | C24   | 1772 | ASP  | C-N   | 6.21  | 1.42        | 1.33     |
| 10  | C24   | 1831 | GLU  | C-N   | -6.20 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A32   | 144  | LYS  | C-N   | 6.20  | 1.42        | 1.33     |
| 11  | A32   | 697  | ASN  | C-N   | -6.20 | 1.26        | 1.33     |
| 23  | J16   | 588  | GLU  | C-N   | -6.20 | 1.26        | 1.33     |
| 1   | R     | 1389 | GLN  | C-N   | -6.20 | 1.25        | 1.33     |
| 5   | P16   | 623  | ALA  | C-N   | 6.20  | 1.42        | 1.33     |
| 10  | C24   | 1367 | ALA  | C-N   | 6.20  | 1.42        | 1.33     |
| 5   | P8    | 160  | LYS  | C-N   | 6.20  | 1.42        | 1.33     |
| 13  | V     | 885  | ARG  | C-N   | 6.20  | 1.41        | 1.33     |
| 11  | A16   | 697  | ASN  | C-N   | -6.20 | 1.26        | 1.33     |
| 10  | C32   | 316  | ILE  | C-N   | 6.20  | 1.42        | 1.33     |
| 11  | A24   | 341  | PRO  | C-N   | -6.20 | 1.26        | 1.33     |
| 7   | Q     | 121  | ILE  | C-N   | -6.20 | 1.25        | 1.33     |
| 9   | K     | 606  | GLU  | C-N   | -6.20 | 1.25        | 1.33     |
| 9   | K     | 710  | ILE  | C-N   | -6.20 | 1.25        | 1.33     |
| 10  | C24   | 1768 | ILE  | C-N   | -6.20 | 1.24        | 1.33     |
| 10  | C8    | 316  | ILE  | C-N   | 6.20  | 1.42        | 1.33     |
| 11  | A32   | 341  | PRO  | C-N   | -6.20 | 1.26        | 1.33     |
| 20  | E     | 293  | ASN  | C-N   | -6.20 | 1.25        | 1.33     |
| 11  | A40   | 134  | LYS  | C-N   | 6.19  | 1.41        | 1.33     |
| 22  | I24   | 170  | ALA  | C-N   | -6.19 | 1.25        | 1.33     |
| 1   | R     | 1492 | SER  | C-N   | -6.19 | 1.25        | 1.34     |
| 5   | P     | 213  | LYS  | C-N   | -6.19 | 1.25        | 1.33     |
| 10  | C16   | 1604 | VAL  | C-N   | 6.19  | 1.42        | 1.33     |
| 11  | A24   | 485  | TYR  | C-N   | -6.19 | 1.25        | 1.34     |
| 10  | C     | 923  | PRO  | C-N   | -6.19 | 1.26        | 1.34     |
| 18  | B8    | 1117 | THR  | C-N   | 6.19  | 1.42        | 1.33     |
| 2   | M8    | 515  | PRO  | C-N   | -6.19 | 1.26        | 1.33     |
| 2   | M16   | 821  | THR  | C-N   | -6.19 | 1.25        | 1.34     |
| 5   | P16   | 160  | LYS  | C-N   | 6.19  | 1.42        | 1.33     |
| 10  | C8    | 1367 | ALA  | C-N   | 6.19  | 1.42        | 1.33     |
| 11  | A16   | 485  | TYR  | C-N   | -6.19 | 1.25        | 1.34     |
| 22  | I     | 282  | GLU  | C-N   | -6.19 | 1.25        | 1.33     |
| 20  | E8    | 481  | LEU  | C-N   | -6.19 | 1.25        | 1.33     |
| 7   | Q     | 152  | GLY  | C-N   | -6.19 | 1.25        | 1.33     |
| 5   | P16   | 57   | PRO  | N-CD  | -6.18 | 1.39        | 1.47     |
| 11  | A24   | 647  | GLY  | C-N   | -6.18 | 1.24        | 1.33     |
| 12  | A     | 697  | ASN  | C-N   | -6.18 | 1.26        | 1.33     |
| 10  | C     | 1768 | ILE  | C-N   | -6.18 | 1.24        | 1.33     |
| 10  | C8    | 1768 | ILE  | C-N   | -6.18 | 1.24        | 1.33     |
| 10  | C32   | 280  | SER  | C-N   | -6.18 | 1.25        | 1.33     |
| 12  | A     | 642  | GLY  | C-N   | 6.18  | 1.41        | 1.33     |
| 20  | E     | 255  | ALA  | C-N   | -6.18 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A40   | 495  | THR  | C-N   | -6.18 | 1.25        | 1.33     |
| 22  | I8    | 318  | VAL  | C-N   | -6.18 | 1.25        | 1.33     |
| 10  | C32   | 1367 | ALA  | C-N   | 6.18  | 1.42        | 1.33     |
| 21  | H16   | 255  | LEU  | C-N   | -6.18 | 1.25        | 1.33     |
| 12  | A     | 859  | ARG  | C-N   | -6.18 | 1.24        | 1.33     |
| 20  | E8    | 293  | ASN  | C-N   | -6.18 | 1.25        | 1.33     |
| 2   | M     | 169  | THR  | C-N   | 6.17  | 1.41        | 1.33     |
| 9   | K8    | 580  | ARG  | C-N   | -6.17 | 1.25        | 1.33     |
| 10  | C24   | 923  | PRO  | C-N   | -6.17 | 1.26        | 1.34     |
| 10  | C8    | 451  | GLU  | C-N   | -6.17 | 1.25        | 1.33     |
| 3   | N     | 204  | PRO  | C-N   | 6.17  | 1.41        | 1.33     |
| 1   | R8    | 1492 | SER  | C-N   | -6.17 | 1.25        | 1.34     |
| 10  | C     | 1353 | ASP  | C-N   | 6.17  | 1.42        | 1.33     |
| 20  | E     | 248  | PHE  | C-N   | -6.17 | 1.25        | 1.33     |
| 14  | W     | 762  | GLN  | C-N   | 6.17  | 1.42        | 1.33     |
| 21  | H8    | 324  | LEU  | C-N   | -6.17 | 1.26        | 1.33     |
| 10  | C32   | 1604 | VAL  | C-N   | 6.17  | 1.42        | 1.33     |
| 9   | K     | 1038 | SER  | C-N   | -6.17 | 1.25        | 1.33     |
| 10  | C     | 316  | ILE  | C-N   | 6.17  | 1.42        | 1.33     |
| 19  | 4     | 37   | VAL  | C-N   | -6.17 | 1.24        | 1.33     |
| 22  | I     | 170  | ALA  | C-N   | -6.17 | 1.25        | 1.33     |
| 7   | Q8    | 152  | GLY  | C-N   | -6.17 | 1.25        | 1.33     |
| 9   | K8    | 642  | ARG  | C-N   | 6.17  | 1.41        | 1.33     |
| 19  | 48    | 16   | ASN  | C-N   | -6.17 | 1.24        | 1.33     |
| 2   | M16   | 515  | PRO  | C-N   | -6.17 | 1.26        | 1.33     |
| 11  | A32   | 36   | ASN  | C-N   | -6.16 | 1.25        | 1.33     |
| 10  | C16   | 1159 | SER  | C-N   | -6.16 | 1.24        | 1.33     |
| 10  | C     | 1132 | SER  | C-N   | -6.16 | 1.26        | 1.34     |
| 18  | B     | 193  | LYS  | C-N   | 6.16  | 1.42        | 1.33     |
| 19  | 48    | 37   | VAL  | C-N   | -6.16 | 1.24        | 1.33     |
| 20  | E8    | 251  | PRO  | N-CD  | -6.16 | 1.39        | 1.47     |
| 1   | R16   | 1214 | ILE  | C-N   | -6.16 | 1.24        | 1.33     |
| 9   | K     | 1019 | ARG  | C-N   | -6.16 | 1.26        | 1.33     |
| 18  | B8    | 193  | LYS  | C-N   | 6.16  | 1.42        | 1.33     |
| 1   | R8    | 1138 | LEU  | C-N   | -6.16 | 1.25        | 1.33     |
| 9   | K     | 935  | GLU  | C-N   | -6.16 | 1.25        | 1.33     |
| 10  | C32   | 1768 | ILE  | C-N   | -6.15 | 1.25        | 1.33     |
| 9   | K8    | 706  | LEU  | C-N   | -6.15 | 1.25        | 1.33     |
| 9   | K8    | 710  | ILE  | C-N   | -6.15 | 1.25        | 1.33     |
| 10  | C     | 280  | SER  | C-N   | -6.15 | 1.25        | 1.33     |
| 10  | C8    | 1831 | GLU  | C-N   | -6.15 | 1.25        | 1.33     |
| 18  | B     | 1419 | LYS  | C-N   | 6.15  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | I16   | 170  | ALA  | C-N   | -6.15 | 1.25        | 1.33     |
| 5   | P     | 64   | ASP  | C-N   | -6.15 | 1.25        | 1.33     |
| 9   | K     | 580  | ARG  | C-N   | -6.15 | 1.25        | 1.33     |
| 11  | A32   | 495  | THR  | C-N   | -6.15 | 1.25        | 1.33     |
| 20  | E8    | 255  | ALA  | C-N   | -6.15 | 1.25        | 1.34     |
| 10  | C32   | 923  | PRO  | C-N   | -6.15 | 1.26        | 1.34     |
| 2   | M     | 515  | PRO  | C-N   | -6.15 | 1.26        | 1.33     |
| 5   | P     | 160  | LYS  | C-N   | 6.14  | 1.42        | 1.33     |
| 11  | A16   | 642  | GLY  | C-N   | 6.14  | 1.41        | 1.33     |
| 21  | H8    | 166  | VAL  | C-N   | -6.14 | 1.25        | 1.33     |
| 21  | H24   | 331  | ASP  | C-N   | -6.14 | 1.25        | 1.33     |
| 9   | K     | 1266 | MET  | C-N   | -6.14 | 1.25        | 1.34     |
| 18  | B     | 1645 | GLU  | C-N   | -6.14 | 1.25        | 1.33     |
| 18  | B     | 1954 | LYS  | C-N   | -6.14 | 1.25        | 1.33     |
| 2   | M     | 723  | ASP  | C-N   | 6.14  | 1.42        | 1.33     |
| 10  | C8    | 280  | SER  | C-N   | -6.14 | 1.25        | 1.33     |
| 10  | C32   | 1353 | ASP  | C-N   | 6.14  | 1.42        | 1.33     |
| 12  | A48   | 697  | ASN  | C-N   | -6.14 | 1.26        | 1.33     |
| 2   | M16   | 723  | ASP  | C-N   | 6.13  | 1.42        | 1.33     |
| 10  | C     | 1772 | ASP  | C-N   | 6.13  | 1.42        | 1.33     |
| 9   | K8    | 1038 | SER  | C-N   | -6.13 | 1.25        | 1.33     |
| 21  | H16   | 324  | LEU  | C-N   | -6.13 | 1.26        | 1.33     |
| 2   | M16   | 358  | LEU  | C-N   | -6.13 | 1.26        | 1.33     |
| 5   | P16   | 64   | ASP  | C-N   | -6.13 | 1.25        | 1.33     |
| 15  | J     | 578  | ASN  | C-N   | -6.13 | 1.25        | 1.33     |
| 11  | A16   | 495  | THR  | C-N   | -6.13 | 1.25        | 1.33     |
| 11  | A16   | 647  | GLY  | C-N   | -6.13 | 1.24        | 1.33     |
| 12  | A48   | 495  | THR  | C-N   | -6.13 | 1.25        | 1.33     |
| 18  | B     | 1412 | SER  | C-N   | -6.13 | 1.25        | 1.33     |
| 10  | C16   | 280  | SER  | C-N   | -6.13 | 1.25        | 1.33     |
| 11  | A32   | 485  | TYR  | C-N   | -6.13 | 1.25        | 1.34     |
| 18  | B8    | 1419 | LYS  | C-N   | 6.13  | 1.43        | 1.33     |
| 21  | H     | 324  | LEU  | C-N   | -6.13 | 1.26        | 1.33     |
| 21  | H24   | 255  | LEU  | C-N   | -6.13 | 1.25        | 1.33     |
| 13  | V     | 867  | ASP  | C-N   | -6.13 | 1.24        | 1.33     |
| 15  | J     | 574  | ARG  | C-N   | -6.13 | 1.26        | 1.33     |
| 19  | 4     | 16   | ASN  | C-N   | -6.13 | 1.24        | 1.33     |
| 1   | R     | 1214 | ILE  | C-N   | -6.12 | 1.24        | 1.33     |
| 5   | P     | 20   | GLU  | C-N   | 6.12  | 1.41        | 1.33     |
| 20  | E     | 251  | PRO  | N-CD  | -6.12 | 1.39        | 1.47     |
| 21  | H24   | 166  | VAL  | C-N   | -6.12 | 1.25        | 1.33     |
| 22  | I24   | 282  | GLU  | C-N   | -6.12 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23  | J24   | 588  | GLU  | C-N   | -6.12 | 1.26        | 1.33     |
| 11  | A24   | 495  | THR  | C-N   | -6.12 | 1.25        | 1.33     |
| 22  | I24   | 187  | ASP  | C-N   | -6.12 | 1.25        | 1.33     |
| 9   | K8    | 1266 | MET  | C-N   | -6.12 | 1.25        | 1.34     |
| 19  | 48    | 383  | ALA  | C-N   | -6.12 | 1.25        | 1.33     |
| 10  | C     | 1140 | GLY  | C-N   | 6.12  | 1.42        | 1.33     |
| 10  | C8    | 1567 | LEU  | C-N   | 6.12  | 1.43        | 1.33     |
| 2   | M     | 358  | LEU  | C-N   | -6.12 | 1.26        | 1.33     |
| 2   | M16   | 834  | ASP  | C-N   | -6.12 | 1.25        | 1.33     |
| 10  | C16   | 1768 | ILE  | C-N   | -6.12 | 1.25        | 1.33     |
| 10  | C24   | 280  | SER  | C-N   | -6.12 | 1.25        | 1.33     |
| 10  | C     | 451  | GLU  | C-N   | -6.12 | 1.25        | 1.33     |
| 23  | J32   | 588  | GLU  | C-N   | -6.12 | 1.26        | 1.33     |
| 18  | B     | 508  | ALA  | C-N   | -6.12 | 1.25        | 1.33     |
| 14  | W     | 605  | ASN  | C-N   | -6.12 | 1.24        | 1.33     |
| 5   | P     | 611  | LEU  | C-N   | -6.11 | 1.25        | 1.33     |
| 5   | P8    | 57   | PRO  | N-CD  | -6.11 | 1.39        | 1.47     |
| 10  | C24   | 1159 | SER  | C-N   | -6.11 | 1.24        | 1.33     |
| 10  | C24   | 1163 | LEU  | C-N   | -6.11 | 1.26        | 1.34     |
| 1   | R16   | 1138 | LEU  | C-N   | -6.11 | 1.25        | 1.33     |
| 10  | C16   | 923  | PRO  | C-N   | -6.11 | 1.26        | 1.34     |
| 10  | C24   | 451  | GLU  | C-N   | -6.11 | 1.25        | 1.33     |
| 21  | H     | 331  | ASP  | C-N   | -6.11 | 1.25        | 1.33     |
| 22  | I8    | 187  | ASP  | C-N   | -6.11 | 1.25        | 1.33     |
| 2   | M8    | 169  | THR  | C-N   | 6.11  | 1.41        | 1.33     |
| 5   | P     | 57   | PRO  | N-CD  | -6.11 | 1.39        | 1.47     |
| 10  | C     | 1604 | VAL  | C-N   | 6.11  | 1.42        | 1.33     |
| 18  | B     | 639  | ALA  | C-N   | 6.11  | 1.41        | 1.33     |
| 10  | C24   | 1438 | ASN  | C-N   | -6.10 | 1.28        | 1.33     |
| 1   | R     | 1138 | LEU  | C-N   | -6.10 | 1.25        | 1.33     |
| 2   | M8    | 834  | ASP  | C-N   | -6.10 | 1.25        | 1.33     |
| 5   | P     | 375  | LYS  | C-N   | -6.10 | 1.24        | 1.33     |
| 10  | C8    | 1604 | VAL  | C-N   | 6.10  | 1.42        | 1.33     |
| 21  | H     | 166  | VAL  | C-N   | -6.10 | 1.25        | 1.33     |
| 22  | I8    | 282  | GLU  | C-N   | -6.10 | 1.25        | 1.33     |
| 14  | W     | 648  | ASN  | C-N   | -6.10 | 1.25        | 1.33     |
| 18  | B     | 1323 | ASN  | C-N   | 6.10  | 1.42        | 1.33     |
| 18  | B8    | 508  | ALA  | C-N   | -6.10 | 1.25        | 1.33     |
| 18  | B8    | 1452 | LYS  | C-N   | -6.10 | 1.25        | 1.33     |
| 21  | H24   | 323  | TYR  | C-N   | 6.10  | 1.43        | 1.33     |
| 9   | K8    | 970  | LEU  | C-N   | -6.09 | 1.25        | 1.33     |
| 19  | 48    | 417  | ASP  | C-N   | -6.09 | 1.24        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | N16   | 22   | TYR  | C-N   | 6.09  | 1.40        | 1.33     |
| 9   | K8    | 1272 | GLU  | C-N   | -6.09 | 1.25        | 1.33     |
| 18  | B8    | 601  | HIS  | C-N   | 6.09  | 1.42        | 1.33     |
| 10  | C32   | 1567 | LEU  | C-N   | 6.09  | 1.43        | 1.33     |
| 11  | A40   | 697  | ASN  | C-N   | -6.09 | 1.26        | 1.33     |
| 9   | K     | 706  | LEU  | C-N   | -6.09 | 1.25        | 1.33     |
| 18  | B     | 1452 | LYS  | C-N   | -6.09 | 1.25        | 1.33     |
| 10  | C16   | 1163 | LEU  | C-N   | -6.09 | 1.26        | 1.34     |
| 11  | A40   | 485  | TYR  | C-N   | -6.09 | 1.25        | 1.34     |
| 10  | C8    | 1159 | SER  | C-N   | -6.09 | 1.24        | 1.33     |
| 20  | E8    | 383  | LYS  | C-N   | -6.09 | 1.25        | 1.33     |
| 22  | I     | 187  | ASP  | C-N   | -6.09 | 1.25        | 1.33     |
| 21  | H16   | 166  | VAL  | C-N   | -6.09 | 1.25        | 1.33     |
| 9   | K     | 768  | GLU  | C-N   | -6.08 | 1.25        | 1.33     |
| 10  | C24   | 1567 | LEU  | C-N   | 6.08  | 1.43        | 1.33     |
| 13  | V     | 778  | GLY  | C-N   | -6.08 | 1.25        | 1.33     |
| 12  | A48   | 642  | GLY  | C-N   | 6.08  | 1.41        | 1.33     |
| 5   | P8    | 375  | LYS  | C-N   | -6.08 | 1.24        | 1.33     |
| 10  | C32   | 1163 | LEU  | C-N   | -6.08 | 1.26        | 1.34     |
| 18  | B8    | 1272 | TRP  | C-N   | 6.08  | 1.42        | 1.33     |
| 23  | J8    | 588  | GLU  | C-N   | -6.08 | 1.26        | 1.33     |
| 2   | M8    | 467  | ILE  | C-N   | -6.08 | 1.25        | 1.33     |
| 10  | C16   | 643  | LEU  | C-N   | 6.08  | 1.42        | 1.33     |
| 18  | B8    | 291  | GLY  | C-N   | 6.08  | 1.40        | 1.33     |
| 10  | C32   | 451  | GLU  | C-N   | -6.08 | 1.25        | 1.33     |
| 2   | M8    | 723  | ASP  | C-N   | 6.08  | 1.42        | 1.33     |
| 10  | C16   | 313  | ILE  | C-N   | 6.08  | 1.41        | 1.33     |
| 18  | B8    | 991  | ASP  | C-N   | 6.08  | 1.42        | 1.33     |
| 18  | B8    | 1412 | SER  | C-N   | -6.08 | 1.25        | 1.33     |
| 21  | H     | 328  | THR  | C-N   | -6.08 | 1.24        | 1.33     |
| 18  | B     | 601  | HIS  | C-N   | 6.07  | 1.42        | 1.33     |
| 18  | B     | 1615 | LYS  | C-N   | -6.07 | 1.25        | 1.34     |
| 22  | I24   | 267  | VAL  | C-N   | -6.07 | 1.25        | 1.33     |
| 10  | C16   | 1168 | PRO  | C-N   | 6.07  | 1.44        | 1.33     |
| 11  | A24   | 642  | GLY  | C-N   | 6.07  | 1.41        | 1.33     |
| 10  | C16   | 1438 | ASN  | C-N   | -6.07 | 1.28        | 1.33     |
| 22  | I16   | 187  | ASP  | C-N   | -6.07 | 1.25        | 1.33     |
| 2   | M8    | 585  | GLY  | C-N   | 6.07  | 1.42        | 1.34     |
| 10  | C16   | 572  | ILE  | C-N   | -6.07 | 1.25        | 1.33     |
| 18  | B8    | 1615 | LYS  | C-N   | -6.07 | 1.25        | 1.34     |
| 20  | E     | 383  | LYS  | C-N   | -6.07 | 1.25        | 1.33     |
| 19  | 48    | 176  | PRO  | C-N   | -6.07 | 1.23        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | H24   | 328  | THR  | C-N   | -6.07 | 1.24        | 1.33     |
| 10  | C32   | 1159 | SER  | C-N   | -6.07 | 1.24        | 1.33     |
| 3   | N     | 22   | TYR  | C-N   | 6.06  | 1.40        | 1.33     |
| 7   | Q     | 28   | ALA  | C-N   | 6.06  | 1.41        | 1.33     |
| 5   | P8    | 676  | GLN  | C-N   | -6.06 | 1.25        | 1.33     |
| 9   | K8    | 834  | VAL  | C-N   | -6.06 | 1.26        | 1.33     |
| 10  | C16   | 1567 | LEU  | C-N   | 6.06  | 1.43        | 1.33     |
| 10  | C8    | 60   | LYS  | C-N   | -6.06 | 1.25        | 1.33     |
| 18  | B     | 486  | PHE  | C-N   | -6.06 | 1.25        | 1.33     |
| 21  | H24   | 324  | LEU  | C-N   | -6.06 | 1.26        | 1.33     |
| 12  | A48   | 485  | TYR  | C-N   | -6.06 | 1.25        | 1.34     |
| 9   | K8    | 935  | GLU  | C-N   | -6.06 | 1.25        | 1.33     |
| 5   | P16   | 375  | LYS  | C-N   | -6.06 | 1.24        | 1.33     |
| 11  | A40   | 65   | ARG  | C-N   | -6.06 | 1.26        | 1.33     |
| 11  | A16   | 154  | ILE  | C-N   | 6.06  | 1.42        | 1.33     |
| 3   | N8    | 22   | TYR  | C-N   | 6.06  | 1.40        | 1.33     |
| 5   | P16   | 631  | VAL  | C-N   | -6.06 | 1.26        | 1.33     |
| 19  | 4     | 383  | ALA  | C-N   | -6.06 | 1.25        | 1.33     |
| 2   | M     | 585  | GLY  | C-N   | 6.06  | 1.42        | 1.34     |
| 11  | A24   | 635  | TYR  | C-N   | -6.06 | 1.25        | 1.33     |
| 10  | C     | 643  | LEU  | C-N   | 6.06  | 1.42        | 1.33     |
| 10  | C32   | 1140 | GLY  | C-N   | 6.06  | 1.42        | 1.33     |
| 5   | P     | 676  | GLN  | C-N   | -6.05 | 1.26        | 1.33     |
| 9   | K     | 970  | LEU  | C-N   | -6.05 | 1.26        | 1.33     |
| 10  | C16   | 1140 | GLY  | C-N   | 6.05  | 1.42        | 1.33     |
| 18  | B     | 1908 | TYR  | C-N   | -6.05 | 1.25        | 1.33     |
| 18  | B8    | 326  | PRO  | N-CD  | 6.05  | 1.56        | 1.47     |
| 18  | B8    | 1323 | ASN  | C-N   | 6.05  | 1.41        | 1.33     |
| 21  | H24   | 136  | TYR  | C-N   | 6.05  | 1.42        | 1.33     |
| 21  | H16   | 136  | TYR  | C-N   | 6.05  | 1.42        | 1.33     |
| 5   | P     | 486  | CYS  | C-N   | -6.05 | 1.25        | 1.33     |
| 15  | J     | 583  | LEU  | C-N   | -6.05 | 1.25        | 1.33     |
| 10  | C8    | 1140 | GLY  | C-N   | 6.05  | 1.42        | 1.33     |
| 18  | B     | 326  | PRO  | N-CD  | 6.05  | 1.56        | 1.47     |
| 19  | 4     | 176  | PRO  | C-N   | -6.05 | 1.24        | 1.33     |
| 20  | E8    | 414  | MET  | C-N   | -6.05 | 1.25        | 1.33     |
| 5   | P8    | 486  | CYS  | C-N   | -6.05 | 1.25        | 1.33     |
| 5   | P8    | 631  | VAL  | C-N   | -6.05 | 1.26        | 1.33     |
| 10  | C8    | 1353 | ASP  | C-N   | 6.05  | 1.42        | 1.33     |
| 22  | I     | 267  | VAL  | C-N   | -6.05 | 1.26        | 1.33     |
| 10  | C8    | 1772 | ASP  | C-N   | 6.05  | 1.42        | 1.33     |
| 10  | C32   | 1168 | PRO  | C-N   | 6.05  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 572  | ILE  | C-N   | -6.05 | 1.25        | 1.33     |
| 10  | C8    | 643  | LEU  | C-N   | 6.05  | 1.42        | 1.33     |
| 11  | A32   | 642  | GLY  | C-N   | 6.05  | 1.41        | 1.33     |
| 18  | B     | 291  | GLY  | C-N   | 6.05  | 1.40        | 1.33     |
| 2   | M8    | 517  | PRO  | C-N   | -6.04 | 1.26        | 1.33     |
| 5   | P16   | 676  | GLN  | C-N   | -6.04 | 1.26        | 1.33     |
| 18  | B8    | 1811 | PRO  | C-N   | -6.04 | 1.25        | 1.33     |
| 1   | R8    | 1214 | ILE  | C-N   | -6.04 | 1.24        | 1.33     |
| 21  | H8    | 301  | ARG  | C-N   | -6.04 | 1.26        | 1.33     |
| 2   | M     | 517  | PRO  | C-N   | -6.04 | 1.26        | 1.33     |
| 2   | M     | 834  | ASP  | C-N   | -6.04 | 1.25        | 1.33     |
| 5   | P     | 623  | ALA  | C-N   | 6.04  | 1.42        | 1.33     |
| 18  | B     | 67   | SER  | C-N   | -6.04 | 1.25        | 1.34     |
| 19  | 4     | 417  | ASP  | C-N   | -6.04 | 1.24        | 1.33     |
| 21  | H16   | 323  | TYR  | C-N   | 6.04  | 1.43        | 1.33     |
| 10  | C32   | 643  | LEU  | C-N   | 6.04  | 1.42        | 1.33     |
| 9   | K8    | 1031 | LEU  | C-N   | -6.04 | 1.25        | 1.33     |
| 10  | C16   | 302  | ALA  | C-N   | 6.04  | 1.42        | 1.33     |
| 11  | A16   | 635  | TYR  | C-N   | -6.04 | 1.25        | 1.33     |
| 5   | P16   | 300  | SER  | C-N   | -6.04 | 1.24        | 1.33     |
| 12  | A     | 485  | TYR  | C-N   | -6.04 | 1.25        | 1.34     |
| 20  | E     | 414  | MET  | C-N   | -6.04 | 1.25        | 1.33     |
| 2   | M16   | 169  | THR  | C-N   | 6.04  | 1.41        | 1.33     |
| 2   | M16   | 467  | ILE  | C-N   | -6.04 | 1.25        | 1.33     |
| 15  | J     | 560  | ARG  | C-N   | -6.04 | 1.26        | 1.33     |
| 10  | C     | 1159 | SER  | C-N   | -6.04 | 1.24        | 1.33     |
| 21  | H16   | 252  | ARG  | C-N   | -6.04 | 1.26        | 1.33     |
| 11  | A40   | 647  | GLY  | C-N   | -6.03 | 1.24        | 1.33     |
| 21  | H     | 136  | TYR  | C-N   | 6.03  | 1.42        | 1.33     |
| 21  | H16   | 331  | ASP  | C-N   | -6.03 | 1.26        | 1.33     |
| 1   | R16   | 1492 | SER  | C-N   | -6.03 | 1.25        | 1.34     |
| 5   | P     | 300  | SER  | C-N   | -6.03 | 1.24        | 1.33     |
| 10  | C8    | 1414 | ASP  | C-N   | -6.03 | 1.24        | 1.33     |
| 2   | M16   | 517  | PRO  | C-N   | -6.03 | 1.26        | 1.33     |
| 5   | P     | 631  | VAL  | C-N   | -6.03 | 1.26        | 1.33     |
| 11  | A16   | 65   | ARG  | C-N   | -6.03 | 1.26        | 1.33     |
| 10  | C     | 302  | ALA  | C-N   | 6.03  | 1.42        | 1.33     |
| 21  | H8    | 323  | TYR  | C-N   | 6.03  | 1.43        | 1.33     |
| 21  | H24   | 301  | ARG  | C-N   | -6.03 | 1.26        | 1.33     |
| 5   | P8    | 611  | LEU  | C-N   | -6.03 | 1.26        | 1.33     |
| 9   | K     | 1272 | GLU  | C-N   | -6.03 | 1.25        | 1.33     |
| 10  | C     | 572  | ILE  | C-N   | -6.02 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | R     | 1124 | TRP  | C-N   | -6.02 | 1.26        | 1.33     |
| 17  | F     | 77   | TYR  | C-N   | 6.02  | 1.42        | 1.33     |
| 18  | B     | 428  | GLN  | C-N   | -6.02 | 1.24        | 1.33     |
| 18  | B     | 1631 | VAL  | C-N   | -6.02 | 1.25        | 1.33     |
| 9   | K8    | 589  | GLY  | C-N   | -6.02 | 1.25        | 1.33     |
| 7   | Q     | 132  | PHE  | C-N   | -6.02 | 1.25        | 1.33     |
| 5   | P16   | 611  | LEU  | C-N   | -6.02 | 1.26        | 1.33     |
| 11  | A32   | 154  | ILE  | C-N   | 6.02  | 1.42        | 1.33     |
| 10  | C16   | 451  | GLU  | C-N   | -6.02 | 1.25        | 1.33     |
| 10  | C24   | 313  | ILE  | C-N   | 6.01  | 1.41        | 1.33     |
| 10  | C24   | 643  | LEU  | C-N   | 6.01  | 1.42        | 1.33     |
| 9   | K     | 1031 | LEU  | C-N   | -6.01 | 1.25        | 1.33     |
| 11  | A24   | 424  | THR  | C-N   | -6.01 | 1.26        | 1.33     |
| 18  | B     | 1811 | PRO  | C-N   | -6.01 | 1.25        | 1.33     |
| 10  | C     | 313  | ILE  | C-N   | 6.01  | 1.41        | 1.33     |
| 18  | B     | 828  | GLU  | C-N   | 6.01  | 1.41        | 1.33     |
| 18  | B     | 1128 | PRO  | C-N   | -6.01 | 1.25        | 1.33     |
| 10  | C24   | 1168 | PRO  | C-N   | 6.01  | 1.44        | 1.33     |
| 10  | C8    | 1163 | LEU  | C-N   | -6.01 | 1.26        | 1.34     |
| 18  | B8    | 1954 | LYS  | C-N   | -6.01 | 1.25        | 1.33     |
| 21  | H8    | 328  | THR  | C-N   | -6.00 | 1.24        | 1.33     |
| 10  | C32   | 313  | ILE  | C-N   | 6.00  | 1.41        | 1.33     |
| 10  | C32   | 1401 | THR  | C-N   | -6.00 | 1.26        | 1.33     |
| 10  | C16   | 1312 | SER  | C-N   | -6.00 | 1.25        | 1.33     |
| 14  | W     | 790  | ASP  | C-N   | -6.00 | 1.25        | 1.33     |
| 10  | C8    | 302  | ALA  | C-N   | 6.00  | 1.42        | 1.33     |
| 11  | A32   | 635  | TYR  | C-N   | -6.00 | 1.25        | 1.33     |
| 18  | B     | 1272 | TRP  | C-N   | 6.00  | 1.42        | 1.33     |
| 5   | P     | 251  | LYS  | C-N   | -6.00 | 1.25        | 1.34     |
| 11  | A24   | 65   | ARG  | C-N   | -6.00 | 1.26        | 1.33     |
| 1   | R8    | 1124 | TRP  | C-N   | -6.00 | 1.26        | 1.33     |
| 10  | C     | 60   | LYS  | C-N   | -6.00 | 1.25        | 1.33     |
| 10  | C     | 1567 | LEU  | C-N   | 6.00  | 1.42        | 1.33     |
| 21  | H8    | 331  | ASP  | C-N   | -6.00 | 1.26        | 1.33     |
| 7   | Q8    | 28   | ALA  | C-N   | 6.00  | 1.41        | 1.33     |
| 9   | K     | 834  | VAL  | C-N   | -6.00 | 1.26        | 1.33     |
| 10  | C24   | 1401 | THR  | C-N   | -6.00 | 1.26        | 1.33     |
| 21  | H16   | 328  | THR  | C-N   | -6.00 | 1.24        | 1.33     |
| 22  | I16   | 267  | VAL  | C-N   | -6.00 | 1.26        | 1.33     |
| 5   | P8    | 300  | SER  | C-N   | -5.99 | 1.24        | 1.33     |
| 18  | B     | 1894 | LYS  | C-N   | -5.99 | 1.26        | 1.33     |
| 5   | P8    | 623  | ALA  | C-N   | 5.99  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1320 | GLN  | C-N   | 5.99  | 1.41        | 1.33     |
| 1   | R     | 1248 | PRO  | N-CD  | -5.99 | 1.39        | 1.47     |
| 11  | A40   | 635  | TYR  | C-N   | -5.99 | 1.25        | 1.33     |
| 18  | B8    | 1128 | PRO  | C-N   | -5.99 | 1.25        | 1.33     |
| 21  | H8    | 136  | TYR  | C-N   | 5.99  | 1.42        | 1.33     |
| 2   | M8    | 358  | LEU  | C-N   | -5.99 | 1.26        | 1.33     |
| 10  | C16   | 1401 | THR  | C-N   | -5.99 | 1.26        | 1.33     |
| 11  | A32   | 65   | ARG  | C-N   | -5.99 | 1.26        | 1.33     |
| 10  | C32   | 302  | ALA  | C-N   | 5.99  | 1.42        | 1.33     |
| 10  | C     | 1163 | LEU  | C-N   | -5.99 | 1.26        | 1.34     |
| 2   | M16   | 701  | SER  | C-N   | 5.99  | 1.41        | 1.33     |
| 9   | K8    | 768  | GLU  | C-N   | -5.99 | 1.25        | 1.33     |
| 10  | C8    | 902  | ASP  | C-N   | 5.99  | 1.41        | 1.33     |
| 10  | C32   | 572  | ILE  | C-N   | -5.99 | 1.25        | 1.33     |
| 2   | M16   | 713  | SER  | C-N   | -5.98 | 1.25        | 1.33     |
| 5   | P16   | 486  | CYS  | C-N   | -5.98 | 1.25        | 1.33     |
| 10  | C24   | 1149 | PHE  | C-N   | -5.98 | 1.26        | 1.33     |
| 2   | M16   | 585  | GLY  | C-N   | 5.98  | 1.42        | 1.34     |
| 12  | A     | 635  | TYR  | C-N   | -5.98 | 1.25        | 1.33     |
| 18  | B     | 226  | TYR  | C-N   | 5.98  | 1.42        | 1.33     |
| 18  | B     | 991  | ASP  | C-N   | 5.98  | 1.42        | 1.33     |
| 20  | E     | 195  | ILE  | C-N   | -5.98 | 1.25        | 1.33     |
| 19  | 48    | 302  | GLY  | C-N   | -5.98 | 1.25        | 1.33     |
| 2   | M     | 447  | LEU  | C-N   | -5.98 | 1.25        | 1.33     |
| 9   | K8    | 1150 | GLU  | C-N   | -5.98 | 1.26        | 1.33     |
| 21  | H     | 252  | ARG  | C-N   | -5.98 | 1.26        | 1.33     |
| 5   | P16   | 111  | SER  | C-N   | -5.98 | 1.25        | 1.33     |
| 9   | K8    | 655  | GLN  | C-N   | -5.98 | 1.25        | 1.33     |
| 10  | C     | 1168 | PRO  | C-N   | 5.98  | 1.44        | 1.33     |
| 1   | R16   | 1382 | LYS  | C-N   | 5.98  | 1.41        | 1.33     |
| 17  | F16   | 77   | TYR  | C-N   | 5.98  | 1.42        | 1.33     |
| 20  | E8    | 195  | ILE  | C-N   | -5.98 | 1.25        | 1.33     |
| 1   | R     | 1382 | LYS  | C-N   | 5.97  | 1.41        | 1.33     |
| 9   | K8    | 769  | GLU  | C-N   | -5.97 | 1.26        | 1.33     |
| 11  | A40   | 642  | GLY  | C-N   | 5.97  | 1.41        | 1.33     |
| 10  | C8    | 572  | ILE  | C-N   | -5.97 | 1.25        | 1.33     |
| 18  | B     | 1084 | TYR  | C-N   | -5.97 | 1.25        | 1.33     |
| 18  | B8    | 486  | PHE  | C-N   | -5.97 | 1.25        | 1.33     |
| 5   | P8    | 251  | LYS  | C-N   | -5.97 | 1.25        | 1.34     |
| 11  | A16   | 424  | THR  | C-N   | -5.97 | 1.26        | 1.33     |
| 21  | H     | 301  | ARG  | C-N   | -5.97 | 1.26        | 1.33     |
| 21  | H8    | 364  | GLU  | C-N   | -5.97 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A48   | 635  | TYR  | C-N   | -5.97 | 1.25        | 1.33     |
| 13  | V     | 846  | LEU  | C-N   | -5.97 | 1.26        | 1.33     |
| 10  | C     | 1320 | GLN  | C-N   | 5.97  | 1.41        | 1.33     |
| 10  | C     | 1663 | SER  | C-N   | 5.97  | 1.42        | 1.33     |
| 21  | H     | 323  | TYR  | C-N   | 5.97  | 1.43        | 1.33     |
| 10  | C32   | 1663 | SER  | C-N   | 5.97  | 1.42        | 1.33     |
| 10  | C8    | 1149 | PHE  | C-N   | -5.97 | 1.26        | 1.33     |
| 1   | R8    | 1248 | PRO  | N-CD  | -5.97 | 1.39        | 1.47     |
| 10  | C8    | 1652 | LEU  | C-N   | -5.97 | 1.25        | 1.33     |
| 21  | H16   | 301  | ARG  | C-N   | -5.97 | 1.26        | 1.33     |
| 10  | C24   | 60   | LYS  | C-N   | -5.96 | 1.25        | 1.33     |
| 11  | A16   | 788  | PRO  | C-N   | -5.96 | 1.24        | 1.33     |
| 13  | V     | 735  | ASN  | C-N   | -5.96 | 1.25        | 1.33     |
| 10  | C     | 1312 | SER  | C-N   | -5.96 | 1.25        | 1.33     |
| 10  | C24   | 1663 | SER  | C-N   | 5.96  | 1.42        | 1.33     |
| 17  | F8    | 77   | TYR  | C-N   | 5.96  | 1.42        | 1.33     |
| 19  | 48    | 91   | PRO  | C-N   | -5.96 | 1.25        | 1.33     |
| 2   | M     | 467  | ILE  | C-N   | -5.96 | 1.25        | 1.33     |
| 9   | K     | 589  | GLY  | C-N   | -5.96 | 1.25        | 1.33     |
| 10  | C16   | 60   | LYS  | C-N   | -5.96 | 1.25        | 1.33     |
| 2   | M16   | 842  | ASP  | C-N   | -5.96 | 1.25        | 1.33     |
| 9   | K     | 769  | GLU  | C-N   | -5.96 | 1.26        | 1.33     |
| 10  | C16   | 902  | ASP  | C-N   | 5.96  | 1.41        | 1.33     |
| 11  | A32   | 424  | THR  | C-N   | -5.96 | 1.26        | 1.33     |
| 23  | J24   | 645  | ASP  | C-N   | -5.96 | 1.26        | 1.33     |
| 5   | P     | 23   | PRO  | N-CD  | -5.96 | 1.39        | 1.47     |
| 10  | C24   | 902  | ASP  | C-N   | 5.96  | 1.41        | 1.33     |
| 18  | B8    | 1631 | VAL  | C-N   | -5.96 | 1.25        | 1.33     |
| 18  | B8    | 1908 | TYR  | C-N   | -5.96 | 1.25        | 1.33     |
| 11  | A32   | 788  | PRO  | C-N   | -5.96 | 1.24        | 1.33     |
| 1   | R16   | 1124 | TRP  | C-N   | -5.95 | 1.26        | 1.33     |
| 11  | A40   | 626  | GLU  | C-N   | -5.95 | 1.26        | 1.33     |
| 12  | A     | 788  | PRO  | C-N   | -5.95 | 1.24        | 1.33     |
| 10  | C8    | 313  | ILE  | C-N   | 5.95  | 1.41        | 1.33     |
| 10  | C8    | 1168 | PRO  | C-N   | 5.95  | 1.44        | 1.33     |
| 18  | B8    | 1894 | LYS  | C-N   | -5.95 | 1.26        | 1.33     |
| 19  | 4     | 302  | GLY  | C-N   | -5.95 | 1.25        | 1.33     |
| 10  | C32   | 1522 | ILE  | C-N   | -5.95 | 1.26        | 1.33     |
| 1   | R16   | 1250 | ASP  | C-N   | -5.95 | 1.25        | 1.33     |
| 2   | M16   | 447  | LEU  | C-N   | -5.95 | 1.25        | 1.33     |
| 7   | Q16   | 28   | ALA  | C-N   | 5.95  | 1.41        | 1.33     |
| 10  | C16   | 1149 | PHE  | C-N   | -5.95 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1448 | LEU  | C-N   | -5.95 | 1.25        | 1.33     |
| 10  | C8    | 1512 | GLY  | C-N   | -5.95 | 1.25        | 1.33     |
| 18  | B     | 1778 | ALA  | C-N   | 5.95  | 1.41        | 1.33     |
| 20  | E     | 95   | ARG  | C-N   | -5.95 | 1.25        | 1.33     |
| 21  | H8    | 252  | ARG  | C-N   | -5.95 | 1.26        | 1.33     |
| 5   | P16   | 251  | LYS  | C-N   | -5.94 | 1.25        | 1.34     |
| 2   | M     | 701  | SER  | C-N   | 5.94  | 1.41        | 1.33     |
| 5   | P16   | 560  | VAL  | C-N   | -5.94 | 1.26        | 1.33     |
| 10  | C16   | 980  | ASP  | C-N   | -5.94 | 1.25        | 1.33     |
| 10  | C     | 644  | ASN  | C-N   | 5.94  | 1.41        | 1.33     |
| 10  | C8    | 468  | GLU  | C-N   | -5.94 | 1.25        | 1.33     |
| 18  | B8    | 1084 | TYR  | C-N   | -5.94 | 1.25        | 1.33     |
| 1   | R16   | 1248 | PRO  | N-CD  | -5.94 | 1.39        | 1.47     |
| 10  | C8    | 752  | ASN  | C-N   | -5.94 | 1.26        | 1.33     |
| 19  | 4     | 91   | PRO  | C-N   | -5.94 | 1.25        | 1.33     |
| 10  | C32   | 417  | LEU  | C-N   | 5.94  | 1.42        | 1.33     |
| 10  | C32   | 1312 | SER  | C-N   | -5.94 | 1.25        | 1.33     |
| 7   | Q16   | 132  | PHE  | C-N   | -5.94 | 1.25        | 1.33     |
| 10  | C     | 417  | LEU  | C-N   | 5.94  | 1.42        | 1.33     |
| 1   | R     | 1250 | ASP  | C-N   | -5.94 | 1.25        | 1.33     |
| 2   | M     | 842  | ASP  | C-N   | -5.94 | 1.25        | 1.33     |
| 21  | H24   | 252  | ARG  | C-N   | -5.94 | 1.26        | 1.33     |
| 1   | R8    | 1250 | ASP  | C-N   | -5.94 | 1.25        | 1.33     |
| 9   | K     | 609  | SER  | C-N   | -5.93 | 1.25        | 1.34     |
| 18  | B     | 1872 | ALA  | C-N   | 5.93  | 1.42        | 1.33     |
| 18  | B8    | 1659 | ILE  | C-N   | 5.93  | 1.42        | 1.34     |
| 10  | C32   | 1320 | GLN  | C-N   | 5.93  | 1.41        | 1.33     |
| 2   | M8    | 842  | ASP  | C-N   | -5.93 | 1.25        | 1.33     |
| 13  | V     | 896  | HIS  | C-N   | -5.93 | 1.25        | 1.33     |
| 10  | C     | 1149 | PHE  | C-N   | -5.93 | 1.26        | 1.33     |
| 18  | B8    | 1872 | ALA  | C-N   | 5.93  | 1.42        | 1.33     |
| 2   | M8    | 701  | SER  | C-N   | 5.93  | 1.41        | 1.33     |
| 2   | M16   | 504  | GLN  | C-N   | 5.93  | 1.42        | 1.33     |
| 9   | K     | 1150 | GLU  | C-N   | -5.93 | 1.26        | 1.33     |
| 10  | C24   | 302  | ALA  | C-N   | 5.93  | 1.42        | 1.33     |
| 10  | C24   | 417  | LEU  | C-N   | 5.93  | 1.42        | 1.33     |
| 10  | C24   | 1140 | GLY  | C-N   | 5.93  | 1.41        | 1.33     |
| 18  | B     | 1844 | ARG  | C-N   | -5.93 | 1.26        | 1.34     |
| 19  | 48    | 28   | GLU  | C-N   | -5.93 | 1.26        | 1.33     |
| 2   | M8    | 464  | ALA  | C-N   | 5.93  | 1.41        | 1.33     |
| 5   | P     | 82   | GLU  | C-N   | -5.93 | 1.25        | 1.33     |
| 10  | C     | 902  | ASP  | C-N   | 5.93  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 828  | GLU  | C-N   | 5.92  | 1.41        | 1.33     |
| 10  | C32   | 902  | ASP  | C-N   | 5.92  | 1.41        | 1.33     |
| 10  | C32   | 1149 | PHE  | C-N   | -5.92 | 1.26        | 1.33     |
| 3   | N     | 257  | ASP  | C-N   | -5.92 | 1.25        | 1.33     |
| 2   | M8    | 713  | SER  | C-N   | -5.92 | 1.25        | 1.33     |
| 10  | C24   | 855  | VAL  | C-N   | 5.92  | 1.42        | 1.34     |
| 10  | C24   | 1570 | ASP  | C-N   | -5.92 | 1.25        | 1.33     |
| 18  | B8    | 67   | SER  | C-N   | -5.92 | 1.25        | 1.34     |
| 18  | B8    | 446  | GLY  | C-N   | 5.92  | 1.42        | 1.34     |
| 18  | B8    | 428  | GLN  | C-N   | -5.92 | 1.24        | 1.33     |
| 19  | 48    | 255  | GLY  | C-N   | 5.92  | 1.38        | 1.33     |
| 10  | C32   | 1652 | LEU  | C-N   | -5.92 | 1.25        | 1.33     |
| 10  | C     | 468  | GLU  | C-N   | -5.92 | 1.25        | 1.33     |
| 5   | P     | 111  | SER  | C-N   | -5.92 | 1.25        | 1.33     |
| 10  | C16   | 417  | LEU  | C-N   | 5.92  | 1.42        | 1.33     |
| 22  | I8    | 267  | VAL  | C-N   | -5.92 | 1.26        | 1.33     |
| 11  | A40   | 424  | THR  | C-N   | -5.92 | 1.26        | 1.33     |
| 2   | M     | 164  | HIS  | C-N   | -5.91 | 1.27        | 1.33     |
| 7   | Q8    | 132  | PHE  | C-N   | -5.91 | 1.25        | 1.33     |
| 10  | C16   | 1414 | ASP  | C-N   | -5.91 | 1.25        | 1.33     |
| 10  | C32   | 980  | ASP  | C-N   | -5.91 | 1.25        | 1.33     |
| 10  | C24   | 1506 | LYS  | C-N   | -5.91 | 1.25        | 1.33     |
| 10  | C8    | 417  | LEU  | C-N   | 5.91  | 1.42        | 1.33     |
| 10  | C8    | 980  | ASP  | C-N   | -5.91 | 1.25        | 1.33     |
| 10  | C32   | 1506 | LYS  | C-N   | -5.91 | 1.25        | 1.33     |
| 5   | P16   | 23   | PRO  | N-CD  | -5.91 | 1.39        | 1.47     |
| 10  | C16   | 1663 | SER  | C-N   | 5.91  | 1.42        | 1.33     |
| 10  | C     | 1414 | ASP  | C-N   | -5.91 | 1.25        | 1.33     |
| 18  | B8    | 226  | TYR  | C-N   | 5.91  | 1.42        | 1.33     |
| 2   | M8    | 447  | LEU  | C-N   | -5.90 | 1.25        | 1.33     |
| 10  | C16   | 1522 | ILE  | C-N   | -5.90 | 1.26        | 1.33     |
| 10  | C     | 1652 | LEU  | C-N   | -5.90 | 1.25        | 1.33     |
| 9   | K     | 655  | GLN  | C-N   | -5.90 | 1.25        | 1.33     |
| 20  | E8    | 95   | ARG  | C-N   | -5.90 | 1.25        | 1.33     |
| 2   | M     | 360  | LEU  | C-N   | -5.90 | 1.26        | 1.33     |
| 10  | C8    | 1320 | GLN  | C-N   | 5.90  | 1.41        | 1.33     |
| 19  | 4     | 28   | GLU  | C-N   | -5.90 | 1.26        | 1.33     |
| 3   | N     | 280  | ASN  | C-N   | -5.89 | 1.25        | 1.33     |
| 2   | M16   | 205  | CYS  | C-N   | 5.89  | 1.41        | 1.33     |
| 3   | N16   | 171  | GLY  | C-N   | 5.89  | 1.41        | 1.33     |
| 10  | C24   | 1312 | SER  | C-N   | -5.89 | 1.25        | 1.33     |
| 11  | A40   | 726  | ASN  | C-N   | -5.89 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | I16   | 176  | ALA  | C-N   | -5.89 | 1.26        | 1.33     |
| 5   | P8    | 111  | SER  | C-N   | -5.89 | 1.25        | 1.33     |
| 14  | W     | 680  | ARG  | C-N   | -5.89 | 1.26        | 1.33     |
| 2   | M8    | 205  | CYS  | C-N   | 5.89  | 1.41        | 1.33     |
| 2   | M     | 713  | SER  | C-N   | -5.89 | 1.25        | 1.33     |
| 2   | M16   | 360  | LEU  | C-N   | -5.89 | 1.26        | 1.33     |
| 2   | M16   | 464  | ALA  | C-N   | 5.89  | 1.41        | 1.33     |
| 11  | A40   | 788  | PRO  | C-N   | -5.89 | 1.24        | 1.33     |
| 13  | V     | 734  | ILE  | C-N   | -5.89 | 1.26        | 1.33     |
| 15  | J     | 542  | THR  | C-N   | -5.89 | 1.25        | 1.33     |
| 17  | F24   | 77   | TYR  | C-N   | 5.89  | 1.42        | 1.33     |
| 10  | C32   | 1448 | LEU  | C-N   | -5.89 | 1.25        | 1.33     |
| 2   | M16   | 497  | PRO  | N-CD  | 5.88  | 1.55        | 1.47     |
| 18  | B8    | 1844 | ARG  | C-N   | -5.88 | 1.26        | 1.34     |
| 10  | C32   | 60   | LYS  | C-N   | -5.88 | 1.26        | 1.33     |
| 10  | C     | 1288 | VAL  | C-N   | 5.88  | 1.42        | 1.33     |
| 1   | R8    | 1382 | LYS  | C-N   | 5.88  | 1.41        | 1.33     |
| 9   | K     | 1210 | SER  | C-N   | -5.88 | 1.26        | 1.33     |
| 10  | C24   | 1414 | ASP  | C-N   | -5.88 | 1.25        | 1.33     |
| 10  | C8    | 640  | GLN  | C-N   | 5.88  | 1.41        | 1.33     |
| 21  | H24   | 364  | GLU  | C-N   | -5.88 | 1.26        | 1.33     |
| 2   | M     | 327  | SER  | C-N   | -5.88 | 1.25        | 1.33     |
| 10  | C     | 1401 | THR  | C-N   | -5.88 | 1.26        | 1.33     |
| 10  | C8    | 1448 | LEU  | C-N   | -5.88 | 1.25        | 1.33     |
| 18  | B8    | 1418 | ALA  | C-N   | 5.88  | 1.42        | 1.33     |
| 18  | B8    | 1778 | ALA  | C-N   | 5.88  | 1.41        | 1.33     |
| 9   | K8    | 1210 | SER  | C-N   | -5.88 | 1.26        | 1.33     |
| 10  | C32   | 1414 | ASP  | C-N   | -5.88 | 1.25        | 1.33     |
| 10  | C24   | 980  | ASP  | C-N   | -5.87 | 1.25        | 1.33     |
| 10  | C     | 980  | ASP  | C-N   | -5.87 | 1.25        | 1.33     |
| 10  | C8    | 1296 | CYS  | C-N   | 5.87  | 1.41        | 1.33     |
| 10  | C8    | 1570 | ASP  | C-N   | -5.87 | 1.25        | 1.33     |
| 19  | 4     | 210  | GLN  | C-N   | -5.87 | 1.25        | 1.33     |
| 2   | M     | 205  | CYS  | C-N   | 5.87  | 1.41        | 1.33     |
| 10  | C24   | 1288 | VAL  | C-N   | 5.87  | 1.42        | 1.33     |
| 10  | C8    | 1522 | ILE  | C-N   | -5.87 | 1.26        | 1.33     |
| 2   | M8    | 164  | HIS  | C-N   | -5.87 | 1.27        | 1.33     |
| 10  | C16   | 985  | LYS  | C-N   | -5.87 | 1.25        | 1.34     |
| 10  | C16   | 1320 | GLN  | C-N   | 5.87  | 1.41        | 1.33     |
| 11  | A16   | 234  | TYR  | C-N   | -5.87 | 1.25        | 1.34     |
| 19  | 4     | 343  | LEU  | C-N   | -5.87 | 1.25        | 1.33     |
| 20  | E     | 300  | ALA  | C-N   | -5.87 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23  | J8    | 645  | ASP  | C-N   | -5.87 | 1.26        | 1.33     |
| 10  | C16   | 1089 | ALA  | C-N   | -5.86 | 1.26        | 1.33     |
| 10  | C24   | 644  | ASN  | C-N   | 5.86  | 1.41        | 1.33     |
| 10  | C16   | 752  | ASN  | C-N   | -5.86 | 1.26        | 1.33     |
| 10  | C24   | 1522 | ILE  | C-N   | -5.86 | 1.26        | 1.33     |
| 20  | E     | 330  | SER  | C-N   | -5.86 | 1.26        | 1.33     |
| 21  | H16   | 364  | GLU  | C-N   | -5.86 | 1.26        | 1.33     |
| 2   | M8    | 504  | GLN  | C-N   | 5.86  | 1.42        | 1.33     |
| 3   | N8    | 280  | ASN  | C-N   | -5.86 | 1.25        | 1.33     |
| 11  | A24   | 626  | GLU  | C-N   | -5.86 | 1.26        | 1.33     |
| 10  | C24   | 1512 | GLY  | C-N   | -5.86 | 1.25        | 1.33     |
| 10  | C8    | 644  | ASN  | C-N   | 5.86  | 1.41        | 1.33     |
| 18  | B8    | 125  | GLN  | C-N   | -5.86 | 1.25        | 1.34     |
| 23  | J32   | 645  | ASP  | C-N   | -5.86 | 1.26        | 1.33     |
| 6   | O     | 118  | SER  | C-N   | -5.86 | 1.25        | 1.33     |
| 19  | 48    | 347  | ALA  | C-N   | -5.86 | 1.25        | 1.34     |
| 14  | W     | 587  | SER  | C-N   | -5.86 | 1.25        | 1.33     |
| 10  | C8    | 1089 | ALA  | C-N   | -5.86 | 1.26        | 1.33     |
| 10  | C8    | 1454 | ALA  | C-N   | -5.86 | 1.25        | 1.33     |
| 11  | A16   | 626  | GLU  | C-N   | -5.86 | 1.26        | 1.33     |
| 20  | E8    | 330  | SER  | C-N   | -5.86 | 1.26        | 1.33     |
| 22  | I24   | 183  | ILE  | C-N   | -5.86 | 1.26        | 1.33     |
| 12  | A48   | 442  | THR  | C-N   | -5.86 | 1.25        | 1.34     |
| 7   | Q16   | 330  | PRO  | C-N   | -5.86 | 1.25        | 1.33     |
| 13  | V     | 869  | TYR  | C-N   | 5.86  | 1.42        | 1.33     |
| 14  | W     | 616  | GLY  | C-N   | -5.86 | 1.25        | 1.34     |
| 10  | C     | 640  | GLN  | C-N   | 5.86  | 1.41        | 1.33     |
| 10  | C     | 1454 | ALA  | C-N   | -5.86 | 1.25        | 1.33     |
| 10  | C     | 1512 | GLY  | C-N   | -5.86 | 1.25        | 1.33     |
| 10  | C8    | 1506 | LYS  | C-N   | -5.86 | 1.25        | 1.33     |
| 7   | Q8    | 330  | PRO  | C-N   | -5.85 | 1.25        | 1.33     |
| 18  | B     | 446  | GLY  | C-N   | 5.85  | 1.42        | 1.34     |
| 12  | A     | 234  | TYR  | C-N   | -5.85 | 1.25        | 1.34     |
| 10  | C32   | 1826 | ALA  | C-N   | 5.85  | 1.41        | 1.33     |
| 10  | C16   | 644  | ASN  | C-N   | 5.85  | 1.41        | 1.33     |
| 10  | C16   | 1512 | GLY  | C-N   | -5.85 | 1.25        | 1.33     |
| 12  | A48   | 788  | PRO  | C-N   | -5.85 | 1.24        | 1.33     |
| 3   | N     | 143  | SER  | C-N   | 5.85  | 1.42        | 1.33     |
| 2   | M8    | 497  | PRO  | N-CD  | 5.85  | 1.55        | 1.47     |
| 5   | P8    | 82   | GLU  | C-N   | -5.85 | 1.25        | 1.33     |
| 12  | A     | 424  | THR  | C-N   | -5.85 | 1.26        | 1.33     |
| 18  | B     | 177  | ARG  | C-N   | -5.85 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A48   | 234  | TYR  | C-N   | -5.85 | 1.25        | 1.34     |
| 10  | C8    | 1719 | ASP  | C-N   | -5.85 | 1.26        | 1.33     |
| 7   | Q     | 330  | PRO  | C-N   | -5.84 | 1.25        | 1.33     |
| 10  | C16   | 468  | GLU  | C-N   | -5.84 | 1.25        | 1.33     |
| 20  | E8    | 300  | ALA  | C-N   | -5.84 | 1.25        | 1.34     |
| 10  | C32   | 985  | LYS  | C-N   | -5.84 | 1.25        | 1.34     |
| 3   | N     | 171  | GLY  | C-N   | 5.84  | 1.41        | 1.33     |
| 5   | P16   | 225  | GLN  | C-N   | 5.84  | 1.42        | 1.33     |
| 9   | K8    | 801  | ALA  | C-N   | -5.84 | 1.26        | 1.33     |
| 5   | P     | 182  | LYS  | C-N   | -5.84 | 1.25        | 1.33     |
| 12  | A     | 442  | THR  | C-N   | -5.84 | 1.25        | 1.34     |
| 10  | C     | 1570 | ASP  | C-N   | -5.84 | 1.25        | 1.33     |
| 19  | 4     | 255  | GLY  | C-N   | 5.84  | 1.38        | 1.33     |
| 22  | I     | 183  | ILE  | C-N   | -5.84 | 1.26        | 1.33     |
| 18  | B     | 1659 | ILE  | C-N   | 5.84  | 1.41        | 1.34     |
| 2   | M16   | 164  | HIS  | C-N   | -5.84 | 1.27        | 1.33     |
| 18  | B     | 68   | ASP  | C-N   | -5.84 | 1.25        | 1.33     |
| 10  | C16   | 1288 | VAL  | C-N   | 5.83  | 1.41        | 1.33     |
| 18  | B     | 1418 | ALA  | C-N   | 5.83  | 1.41        | 1.33     |
| 22  | I8    | 183  | ILE  | C-N   | -5.83 | 1.26        | 1.33     |
| 1   | R8    | 1201 | LEU  | C-N   | 5.83  | 1.41        | 1.33     |
| 3   | N8    | 171  | GLY  | C-N   | 5.83  | 1.41        | 1.33     |
| 5   | P8    | 23   | PRO  | N-CD  | -5.83 | 1.39        | 1.47     |
| 5   | P16   | 204  | SER  | C-N   | -5.83 | 1.25        | 1.34     |
| 10  | C16   | 1506 | LYS  | C-N   | -5.83 | 1.25        | 1.33     |
| 19  | 48    | 210  | GLN  | C-N   | -5.83 | 1.25        | 1.33     |
| 10  | C32   | 1570 | ASP  | C-N   | -5.83 | 1.25        | 1.33     |
| 2   | M8    | 360  | LEU  | C-N   | -5.83 | 1.26        | 1.33     |
| 2   | M16   | 327  | SER  | C-N   | -5.83 | 1.25        | 1.33     |
| 3   | N8    | 143  | SER  | C-N   | 5.83  | 1.42        | 1.33     |
| 5   | P16   | 20   | GLU  | C-N   | 5.83  | 1.42        | 1.33     |
| 10  | C     | 1522 | ILE  | C-N   | -5.83 | 1.26        | 1.33     |
| 5   | P8    | 560  | VAL  | C-N   | -5.83 | 1.26        | 1.33     |
| 10  | C8    | 1312 | SER  | C-N   | -5.83 | 1.25        | 1.33     |
| 11  | A24   | 788  | PRO  | C-N   | -5.83 | 1.24        | 1.33     |
| 10  | C     | 1089 | ALA  | C-N   | -5.83 | 1.26        | 1.33     |
| 3   | N16   | 143  | SER  | C-N   | 5.83  | 1.42        | 1.33     |
| 5   | P8    | 586  | GLU  | C-N   | -5.83 | 1.26        | 1.33     |
| 11  | A24   | 234  | TYR  | C-N   | -5.83 | 1.25        | 1.34     |
| 10  | C24   | 1652 | LEU  | C-N   | -5.83 | 1.25        | 1.33     |
| 10  | C8    | 1401 | THR  | C-N   | -5.83 | 1.26        | 1.33     |
| 11  | A16   | 726  | ASN  | C-N   | -5.83 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 752  | ASN  | C-N   | -5.83 | 1.26        | 1.33     |
| 2   | M     | 504  | GLN  | C-N   | 5.82  | 1.41        | 1.33     |
| 19  | 4     | 347  | ALA  | C-N   | -5.82 | 1.25        | 1.34     |
| 10  | C32   | 1512 | GLY  | C-N   | -5.82 | 1.26        | 1.33     |
| 3   | N8    | 257  | ASP  | C-N   | -5.82 | 1.25        | 1.33     |
| 5   | P     | 560  | VAL  | C-N   | -5.82 | 1.26        | 1.33     |
| 5   | P8    | 204  | SER  | C-N   | -5.82 | 1.25        | 1.33     |
| 10  | C16   | 408  | GLU  | C-N   | -5.82 | 1.26        | 1.33     |
| 18  | B8    | 1279 | THR  | C-N   | -5.82 | 1.25        | 1.33     |
| 10  | C32   | 644  | ASN  | C-N   | 5.82  | 1.41        | 1.33     |
| 3   | N16   | 257  | ASP  | C-N   | -5.82 | 1.25        | 1.33     |
| 10  | C16   | 113  | LEU  | C-N   | -5.82 | 1.26        | 1.33     |
| 10  | C8    | 1116 | SER  | C-N   | -5.82 | 1.26        | 1.33     |
| 10  | C32   | 1288 | VAL  | C-N   | 5.82  | 1.41        | 1.33     |
| 5   | P16   | 82   | GLU  | C-N   | -5.82 | 1.25        | 1.33     |
| 9   | K8    | 609  | SER  | C-N   | -5.82 | 1.25        | 1.34     |
| 10  | C16   | 1826 | ALA  | C-N   | 5.82  | 1.41        | 1.33     |
| 14  | W     | 783  | LYS  | C-N   | -5.82 | 1.26        | 1.33     |
| 18  | B     | 256  | VAL  | C-N   | -5.82 | 1.25        | 1.33     |
| 18  | B8    | 146  | THR  | C-N   | -5.82 | 1.26        | 1.33     |
| 1   | R16   | 1201 | LEU  | C-N   | 5.82  | 1.41        | 1.33     |
| 3   | N16   | 280  | ASN  | C-N   | -5.82 | 1.25        | 1.33     |
| 11  | A16   | 713  | ASP  | C-N   | -5.82 | 1.26        | 1.33     |
| 23  | J16   | 645  | ASP  | C-N   | -5.82 | 1.26        | 1.33     |
| 1   | R     | 1201 | LEU  | C-N   | 5.81  | 1.41        | 1.33     |
| 2   | M     | 464  | ALA  | C-N   | 5.81  | 1.41        | 1.33     |
| 10  | C24   | 985  | LYS  | C-N   | -5.81 | 1.25        | 1.34     |
| 19  | 4     | 108  | HIS  | C-N   | -5.81 | 1.25        | 1.33     |
| 10  | C16   | 1652 | LEU  | C-N   | -5.81 | 1.25        | 1.33     |
| 19  | 48    | 108  | HIS  | C-N   | -5.81 | 1.25        | 1.33     |
| 23  | J32   | 655  | GLU  | C-N   | -5.81 | 1.26        | 1.33     |
| 5   | P16   | 586  | GLU  | C-N   | -5.81 | 1.26        | 1.33     |
| 18  | B8    | 177  | ARG  | C-N   | -5.81 | 1.26        | 1.33     |
| 9   | K8    | 1237 | PRO  | C-N   | 5.81  | 1.42        | 1.33     |
| 10  | C16   | 1448 | LEU  | C-N   | -5.81 | 1.26        | 1.33     |
| 18  | B     | 107  | ARG  | C-N   | -5.81 | 1.26        | 1.33     |
| 12  | A48   | 424  | THR  | C-N   | -5.81 | 1.26        | 1.33     |
| 5   | P8    | 20   | GLU  | C-N   | 5.81  | 1.41        | 1.33     |
| 10  | C16   | 1570 | ASP  | C-N   | -5.81 | 1.25        | 1.33     |
| 11  | A24   | 4    | ASP  | C-N   | 5.81  | 1.42        | 1.34     |
| 10  | C8    | 1826 | ALA  | C-N   | 5.81  | 1.41        | 1.33     |
| 22  | I16   | 183  | ILE  | C-N   | -5.81 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 24  | D16   | 1440 | PRO  | CA-C  | 5.81  | 1.55        | 1.51     |
| 3   | N     | 39   | GLY  | C-N   | 5.80  | 1.40        | 1.33     |
| 5   | P     | 225  | GLN  | C-N   | 5.80  | 1.42        | 1.33     |
| 10  | C     | 1441 | TYR  | C-N   | 5.80  | 1.42        | 1.33     |
| 10  | C     | 752  | ASN  | C-N   | -5.80 | 1.26        | 1.33     |
| 10  | C8    | 656  | THR  | C-N   | -5.80 | 1.26        | 1.33     |
| 2   | M     | 497  | PRO  | N-CD  | 5.80  | 1.55        | 1.47     |
| 19  | 48    | 343  | LEU  | C-N   | -5.80 | 1.25        | 1.33     |
| 22  | I24   | 176  | ALA  | C-N   | -5.80 | 1.26        | 1.33     |
| 2   | M16   | 431  | ASN  | C-N   | -5.80 | 1.26        | 1.33     |
| 10  | C8    | 1288 | VAL  | C-N   | 5.80  | 1.41        | 1.33     |
| 2   | M8    | 327  | SER  | C-N   | -5.80 | 1.25        | 1.33     |
| 3   | N8    | 39   | GLY  | C-N   | 5.80  | 1.40        | 1.33     |
| 10  | C16   | 640  | GLN  | C-N   | 5.80  | 1.41        | 1.33     |
| 15  | J     | 572  | ASP  | C-N   | -5.80 | 1.26        | 1.33     |
| 21  | H16   | 184  | THR  | C-N   | -5.79 | 1.25        | 1.34     |
| 10  | C16   | 1084 | LYS  | C-N   | -5.79 | 1.25        | 1.33     |
| 11  | A32   | 234  | TYR  | C-N   | -5.79 | 1.25        | 1.34     |
| 22  | I16   | 148  | VAL  | C-N   | 5.79  | 1.42        | 1.33     |
| 10  | C32   | 113  | LEU  | C-N   | -5.79 | 1.26        | 1.33     |
| 2   | M8    | 431  | ASN  | C-N   | -5.79 | 1.26        | 1.33     |
| 5   | P     | 586  | GLU  | C-N   | -5.79 | 1.26        | 1.33     |
| 13  | V     | 738  | ALA  | C-N   | -5.79 | 1.26        | 1.33     |
| 21  | H24   | 213  | SER  | C-N   | -5.79 | 1.26        | 1.33     |
| 10  | C32   | 468  | GLU  | C-N   | -5.79 | 1.25        | 1.33     |
| 5   | P8    | 225  | GLN  | C-N   | 5.79  | 1.42        | 1.33     |
| 12  | A     | 726  | ASN  | C-N   | -5.79 | 1.26        | 1.33     |
| 18  | B     | 467  | ILE  | C-N   | -5.79 | 1.26        | 1.33     |
| 21  | H     | 213  | SER  | C-N   | -5.79 | 1.26        | 1.33     |
| 9   | K8    | 944  | ASN  | C-N   | -5.79 | 1.26        | 1.33     |
| 10  | C     | 1331 | CYS  | C-N   | 5.79  | 1.41        | 1.34     |
| 11  | A16   | 4    | ASP  | C-N   | 5.79  | 1.42        | 1.34     |
| 23  | J24   | 655  | GLU  | C-N   | -5.79 | 1.26        | 1.33     |
| 2   | M     | 468  | HIS  | C-N   | 5.78  | 1.42        | 1.34     |
| 10  | C24   | 468  | GLU  | C-N   | -5.78 | 1.25        | 1.33     |
| 9   | K     | 1197 | THR  | C-N   | -5.78 | 1.26        | 1.33     |
| 11  | A24   | 726  | ASN  | C-N   | -5.78 | 1.26        | 1.33     |
| 23  | J32   | 709  | LYS  | C-N   | -5.78 | 1.26        | 1.33     |
| 21  | H8    | 213  | SER  | C-N   | -5.78 | 1.26        | 1.33     |
| 5   | P16   | 607  | PHE  | C-N   | -5.78 | 1.25        | 1.34     |
| 10  | C24   | 1826 | ALA  | C-N   | 5.78  | 1.41        | 1.33     |
| 11  | A32   | 626  | GLU  | C-N   | -5.78 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 1279 | THR  | C-N   | -5.78 | 1.25        | 1.33     |
| 23  | J16   | 709  | LYS  | C-N   | -5.78 | 1.26        | 1.33     |
| 10  | C32   | 1089 | ALA  | C-N   | -5.78 | 1.26        | 1.33     |
| 23  | J16   | 655  | GLU  | C-N   | -5.78 | 1.26        | 1.33     |
| 3   | N16   | 39   | GLY  | C-N   | 5.78  | 1.40        | 1.33     |
| 5   | P16   | 247  | GLU  | C-N   | -5.78 | 1.26        | 1.33     |
| 9   | K8    | 863  | ASP  | C-N   | -5.78 | 1.26        | 1.33     |
| 18  | B     | 125  | GLN  | C-N   | -5.78 | 1.25        | 1.34     |
| 18  | B8    | 349  | PHE  | C-N   | -5.78 | 1.25        | 1.33     |
| 7   | Q16   | 330  | PRO  | N-CD  | 5.78  | 1.55        | 1.47     |
| 10  | C     | 1793 | VAL  | C-N   | 5.78  | 1.41        | 1.33     |
| 18  | B8    | 107  | ARG  | C-N   | -5.78 | 1.26        | 1.33     |
| 12  | A48   | 726  | ASN  | C-N   | -5.78 | 1.26        | 1.33     |
| 10  | C24   | 408  | GLU  | C-N   | -5.77 | 1.26        | 1.33     |
| 18  | B     | 1350 | ILE  | C-N   | -5.77 | 1.25        | 1.33     |
| 18  | B8    | 467  | ILE  | C-N   | -5.77 | 1.26        | 1.33     |
| 11  | A32   | 442  | THR  | C-N   | -5.77 | 1.25        | 1.34     |
| 21  | H16   | 213  | SER  | C-N   | -5.77 | 1.26        | 1.33     |
| 10  | C32   | 1084 | LYS  | C-N   | -5.77 | 1.25        | 1.33     |
| 2   | M     | 624  | ASP  | C-N   | 5.77  | 1.41        | 1.33     |
| 10  | C     | 1506 | LYS  | C-N   | -5.77 | 1.25        | 1.33     |
| 11  | A32   | 99   | THR  | C-N   | 5.77  | 1.41        | 1.33     |
| 21  | H     | 364  | GLU  | C-N   | -5.77 | 1.26        | 1.33     |
| 9   | K     | 801  | ALA  | C-N   | -5.77 | 1.26        | 1.33     |
| 9   | K     | 863  | ASP  | C-N   | -5.77 | 1.26        | 1.33     |
| 10  | C16   | 327  | ILE  | C-N   | 5.77  | 1.41        | 1.33     |
| 10  | C     | 1826 | ALA  | C-N   | 5.77  | 1.41        | 1.33     |
| 10  | C24   | 1441 | TYR  | C-N   | 5.77  | 1.42        | 1.33     |
| 11  | A40   | 234  | TYR  | C-N   | -5.77 | 1.26        | 1.34     |
| 5   | P8    | 247  | GLU  | C-N   | -5.76 | 1.26        | 1.33     |
| 11  | A32   | 4    | ASP  | C-N   | 5.76  | 1.42        | 1.34     |
| 10  | C32   | 1441 | TYR  | C-N   | 5.76  | 1.42        | 1.33     |
| 10  | C32   | 1454 | ALA  | C-N   | -5.76 | 1.26        | 1.33     |
| 7   | Q     | 330  | PRO  | N-CD  | 5.76  | 1.55        | 1.47     |
| 9   | K     | 978  | GLY  | C-N   | 5.76  | 1.41        | 1.33     |
| 19  | 4     | 382  | ILE  | C-N   | -5.76 | 1.25        | 1.33     |
| 22  | I8    | 176  | ALA  | C-N   | -5.76 | 1.26        | 1.33     |
| 11  | A40   | 442  | THR  | C-N   | -5.76 | 1.26        | 1.34     |
| 15  | J     | 659  | GLU  | C-N   | -5.76 | 1.26        | 1.33     |
| 9   | K     | 1237 | PRO  | C-N   | 5.76  | 1.41        | 1.33     |
| 15  | J     | 706  | ILE  | C-N   | -5.76 | 1.26        | 1.33     |
| 10  | C8    | 408  | GLU  | C-N   | -5.76 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 21  | H8    | 184  | THR  | C-N   | -5.76 | 1.26        | 1.34     |
| 2   | M     | 431  | ASN  | C-N   | -5.76 | 1.26        | 1.33     |
| 10  | C24   | 1339 | VAL  | C-N   | -5.76 | 1.26        | 1.33     |
| 10  | C24   | 1454 | ALA  | C-N   | -5.76 | 1.26        | 1.33     |
| 18  | B8    | 68   | ASP  | C-N   | -5.76 | 1.25        | 1.33     |
| 22  | I     | 176  | ALA  | C-N   | -5.76 | 1.26        | 1.33     |
| 10  | C16   | 656  | THR  | C-N   | -5.75 | 1.26        | 1.33     |
| 10  | C16   | 1296 | CYS  | C-N   | 5.75  | 1.41        | 1.33     |
| 2   | M16   | 415  | ASP  | C-N   | -5.75 | 1.26        | 1.33     |
| 9   | K     | 840  | TRP  | C-N   | -5.75 | 1.26        | 1.33     |
| 10  | C16   | 1116 | SER  | C-N   | -5.75 | 1.26        | 1.33     |
| 11  | A24   | 442  | THR  | C-N   | -5.75 | 1.26        | 1.34     |
| 14  | W     | 705  | HIS  | C-N   | -5.75 | 1.25        | 1.33     |
| 10  | C32   | 1719 | ASP  | C-N   | -5.75 | 1.26        | 1.33     |
| 2   | M8    | 468  | HIS  | C-N   | 5.75  | 1.41        | 1.34     |
| 5   | P8    | 607  | PHE  | C-N   | -5.75 | 1.26        | 1.34     |
| 10  | C16   | 1410 | LEU  | C-N   | 5.75  | 1.40        | 1.33     |
| 20  | E8    | 385  | ASP  | C-N   | -5.75 | 1.26        | 1.34     |
| 21  | H     | 184  | THR  | C-N   | -5.75 | 1.26        | 1.34     |
| 12  | A     | 269  | GLY  | C-N   | -5.75 | 1.24        | 1.33     |
| 20  | E8    | 488  | LEU  | C-N   | -5.75 | 1.26        | 1.33     |
| 23  | J8    | 709  | LYS  | C-N   | -5.75 | 1.26        | 1.33     |
| 5   | P     | 247  | GLU  | C-N   | -5.75 | 1.26        | 1.33     |
| 6   | O8    | 118  | SER  | C-N   | -5.75 | 1.26        | 1.33     |
| 14  | W     | 651  | ARG  | C-N   | -5.75 | 1.26        | 1.33     |
| 10  | C     | 1116 | SER  | C-N   | -5.75 | 1.26        | 1.33     |
| 10  | C     | 1719 | ASP  | C-N   | -5.75 | 1.26        | 1.33     |
| 10  | C32   | 408  | GLU  | C-N   | -5.75 | 1.26        | 1.33     |
| 12  | A48   | 626  | GLU  | C-N   | -5.75 | 1.26        | 1.33     |
| 6   | O16   | 118  | SER  | C-N   | -5.75 | 1.26        | 1.33     |
| 2   | M8    | 551  | GLU  | C-N   | 5.74  | 1.41        | 1.33     |
| 11  | A32   | 269  | GLY  | C-N   | -5.74 | 1.24        | 1.33     |
| 18  | B8    | 1797 | LEU  | C-N   | 5.74  | 1.40        | 1.33     |
| 2   | M16   | 551  | GLU  | C-N   | 5.74  | 1.41        | 1.33     |
| 9   | K8    | 840  | TRP  | C-N   | -5.74 | 1.26        | 1.33     |
| 10  | C24   | 752  | ASN  | C-N   | -5.74 | 1.26        | 1.33     |
| 10  | C     | 1296 | CYS  | C-N   | 5.74  | 1.41        | 1.33     |
| 10  | C8    | 113  | LEU  | C-N   | -5.74 | 1.26        | 1.33     |
| 19  | 48    | 76   | THR  | C-N   | 5.74  | 1.41        | 1.33     |
| 5   | P8    | 182  | LYS  | C-N   | -5.74 | 1.25        | 1.33     |
| 5   | P16   | 412  | GLU  | C-N   | -5.74 | 1.26        | 1.33     |
| 18  | B8    | 256  | VAL  | C-N   | -5.74 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 20  | E     | 488  | LEU  | C-N   | -5.74 | 1.26        | 1.33     |
| 11  | A32   | 726  | ASN  | C-N   | -5.74 | 1.26        | 1.33     |
| 2   | M8    | 624  | ASP  | C-N   | 5.74  | 1.41        | 1.33     |
| 18  | B8    | 249  | TYR  | C-N   | -5.74 | 1.25        | 1.33     |
| 21  | H8    | 357  | LYS  | C-N   | -5.74 | 1.26        | 1.33     |
| 5   | P     | 204  | SER  | C-N   | -5.73 | 1.26        | 1.33     |
| 2   | M16   | 468  | HIS  | C-N   | 5.73  | 1.41        | 1.34     |
| 7   | Q8    | 330  | PRO  | N-CD  | 5.73  | 1.55        | 1.47     |
| 10  | C24   | 654  | PRO  | N-CD  | -5.73 | 1.39        | 1.47     |
| 20  | E     | 385  | ASP  | C-N   | -5.73 | 1.26        | 1.34     |
| 10  | C16   | 1719 | ASP  | C-N   | -5.73 | 1.26        | 1.33     |
| 10  | C     | 750  | TYR  | C-N   | -5.73 | 1.26        | 1.33     |
| 11  | A32   | 713  | ASP  | C-N   | -5.73 | 1.26        | 1.33     |
| 18  | B     | 146  | THR  | C-N   | -5.73 | 1.26        | 1.33     |
| 19  | 4     | 76   | THR  | C-N   | 5.73  | 1.41        | 1.33     |
| 9   | K8    | 1197 | THR  | C-N   | -5.73 | 1.26        | 1.33     |
| 12  | A     | 285  | GLN  | C-N   | -5.73 | 1.26        | 1.33     |
| 9   | K     | 944  | ASN  | C-N   | -5.73 | 1.26        | 1.33     |
| 22  | I     | 148  | VAL  | C-N   | 5.73  | 1.42        | 1.33     |
| 19  | 48    | 292  | SER  | C-N   | -5.73 | 1.25        | 1.33     |
| 15  | J     | 643  | THR  | C-N   | -5.72 | 1.26        | 1.33     |
| 10  | C     | 1448 | LEU  | C-N   | -5.72 | 1.26        | 1.33     |
| 18  | B     | 1249 | LEU  | C-N   | 5.72  | 1.42        | 1.33     |
| 18  | B     | 1797 | LEU  | C-N   | 5.72  | 1.40        | 1.33     |
| 3   | N16   | 225  | PRO  | C-N   | -5.72 | 1.25        | 1.33     |
| 10  | C24   | 640  | GLN  | C-N   | 5.72  | 1.41        | 1.33     |
| 21  | H24   | 184  | THR  | C-N   | -5.72 | 1.26        | 1.34     |
| 10  | C32   | 726  | GLU  | C-N   | 5.72  | 1.42        | 1.33     |
| 10  | C24   | 656  | THR  | C-N   | -5.72 | 1.26        | 1.33     |
| 3   | N8    | 225  | PRO  | C-N   | -5.72 | 1.25        | 1.33     |
| 10  | C16   | 1441 | TYR  | C-N   | 5.72  | 1.42        | 1.33     |
| 20  | E     | 441  | ARG  | C-N   | -5.72 | 1.25        | 1.33     |
| 10  | C     | 327  | ILE  | C-N   | 5.72  | 1.41        | 1.33     |
| 19  | 48    | 370  | SER  | C-N   | -5.72 | 1.25        | 1.33     |
| 10  | C32   | 640  | GLN  | C-N   | 5.72  | 1.41        | 1.33     |
| 10  | C24   | 113  | LEU  | C-N   | -5.71 | 1.26        | 1.33     |
| 10  | C24   | 1296 | CYS  | C-N   | 5.71  | 1.41        | 1.33     |
| 10  | C     | 408  | GLU  | C-N   | -5.71 | 1.26        | 1.33     |
| 19  | 48    | 382  | ILE  | C-N   | -5.71 | 1.25        | 1.33     |
| 10  | C32   | 1331 | CYS  | C-N   | 5.71  | 1.41        | 1.34     |
| 5   | P16   | 182  | LYS  | C-N   | -5.71 | 1.25        | 1.33     |
| 21  | H     | 357  | LYS  | C-N   | -5.71 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K8    | 978  | GLY  | C-N   | 5.71  | 1.41        | 1.33     |
| 12  | A     | 626  | GLU  | C-N   | -5.71 | 1.26        | 1.33     |
| 2   | M8    | 415  | ASP  | C-N   | -5.71 | 1.26        | 1.33     |
| 2   | M8    | 817  | GLU  | C-N   | -5.71 | 1.26        | 1.34     |
| 10  | C16   | 1454 | ALA  | C-N   | -5.71 | 1.26        | 1.33     |
| 10  | C24   | 1511 | VAL  | C-N   | 5.71  | 1.40        | 1.33     |
| 20  | E8    | 441  | ARG  | C-N   | -5.71 | 1.25        | 1.33     |
| 19  | 4     | 370  | SER  | C-N   | -5.71 | 1.25        | 1.33     |
| 10  | C32   | 1296 | CYS  | C-N   | 5.71  | 1.41        | 1.33     |
| 2   | M8    | 256  | HIS  | C-N   | -5.71 | 1.25        | 1.33     |
| 11  | A32   | 111  | MET  | C-N   | -5.71 | 1.26        | 1.33     |
| 10  | C32   | 327  | ILE  | C-N   | 5.71  | 1.41        | 1.33     |
| 11  | A16   | 99   | THR  | C-N   | 5.70  | 1.41        | 1.33     |
| 18  | B8    | 1350 | ILE  | C-N   | -5.70 | 1.25        | 1.33     |
| 19  | 48    | 52   | SER  | C-N   | -5.70 | 1.25        | 1.33     |
| 10  | C32   | 1197 | GLN  | C-N   | -5.70 | 1.26        | 1.33     |
| 13  | V     | 898  | LEU  | C-N   | 5.70  | 1.41        | 1.33     |
| 23  | J8    | 655  | GLU  | C-N   | -5.70 | 1.26        | 1.33     |
| 10  | C16   | 1331 | CYS  | C-N   | 5.70  | 1.41        | 1.34     |
| 11  | A16   | 111  | MET  | C-N   | -5.70 | 1.26        | 1.33     |
| 19  | 4     | 52   | SER  | C-N   | -5.70 | 1.25        | 1.33     |
| 3   | N     | 44   | GLY  | C-N   | 5.70  | 1.37        | 1.33     |
| 21  | H16   | 357  | LYS  | C-N   | -5.70 | 1.26        | 1.33     |
| 2   | M     | 551  | GLU  | C-N   | 5.69  | 1.41        | 1.33     |
| 2   | M8    | 338  | ASN  | C-N   | 5.69  | 1.40        | 1.33     |
| 5   | P     | 287  | MET  | C-N   | 5.69  | 1.39        | 1.33     |
| 9   | K     | 632  | ASP  | C-N   | -5.69 | 1.25        | 1.33     |
| 10  | C8    | 1793 | VAL  | C-N   | 5.69  | 1.41        | 1.33     |
| 21  | H16   | 319  | GLY  | C-N   | -5.69 | 1.25        | 1.33     |
| 9   | K8    | 632  | ASP  | C-N   | -5.69 | 1.25        | 1.33     |
| 10  | C8    | 327  | ILE  | C-N   | 5.69  | 1.41        | 1.33     |
| 18  | B     | 181  | SER  | C-N   | -5.69 | 1.26        | 1.33     |
| 10  | C32   | 1339 | VAL  | C-N   | -5.69 | 1.26        | 1.33     |
| 10  | C16   | 1511 | VAL  | C-N   | 5.69  | 1.40        | 1.33     |
| 10  | C24   | 1089 | ALA  | C-N   | -5.69 | 1.26        | 1.33     |
| 11  | A40   | 4    | ASP  | C-N   | 5.69  | 1.41        | 1.34     |
| 11  | A16   | 442  | THR  | C-N   | -5.69 | 1.26        | 1.34     |
| 18  | B     | 249  | TYR  | C-N   | -5.69 | 1.25        | 1.33     |
| 22  | I     | 180  | GLU  | C-N   | -5.69 | 1.26        | 1.33     |
| 10  | C8    | 1197 | GLN  | C-N   | -5.69 | 1.26        | 1.33     |
| 10  | C8    | 1393 | SER  | C-N   | 5.69  | 1.41        | 1.33     |
| 5   | P     | 607  | PHE  | C-N   | -5.69 | 1.26        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1116 | SER  | C-N   | -5.69 | 1.26        | 1.33     |
| 10  | C     | 113  | LEU  | C-N   | -5.68 | 1.26        | 1.33     |
| 10  | C8    | 1331 | CYS  | C-N   | 5.68  | 1.41        | 1.34     |
| 10  | C16   | 726  | GLU  | C-N   | 5.68  | 1.42        | 1.33     |
| 10  | C16   | 1339 | VAL  | C-N   | -5.68 | 1.26        | 1.33     |
| 11  | A40   | 713  | ASP  | C-N   | -5.68 | 1.26        | 1.33     |
| 18  | B8    | 1366 | LYS  | C-N   | -5.68 | 1.26        | 1.33     |
| 22  | I16   | 180  | GLU  | C-N   | -5.68 | 1.26        | 1.33     |
| 24  | D32   | 1440 | PRO  | CA-C  | 5.68  | 1.55        | 1.51     |
| 10  | C32   | 1116 | SER  | C-N   | -5.68 | 1.26        | 1.33     |
| 10  | C32   | 1793 | VAL  | C-N   | 5.68  | 1.41        | 1.33     |
| 11  | A24   | 269  | GLY  | C-N   | -5.68 | 1.24        | 1.33     |
| 15  | J     | 586  | GLU  | C-N   | -5.68 | 1.26        | 1.33     |
| 3   | N     | 225  | PRO  | C-N   | -5.68 | 1.25        | 1.33     |
| 10  | C16   | 1393 | SER  | C-N   | 5.68  | 1.41        | 1.33     |
| 2   | M16   | 817  | GLU  | C-N   | -5.68 | 1.26        | 1.34     |
| 6   | O8    | 105  | ASN  | C-N   | -5.68 | 1.26        | 1.34     |
| 10  | C     | 422  | THR  | C-N   | -5.68 | 1.25        | 1.33     |
| 18  | B8    | 1379 | VAL  | C-N   | 5.68  | 1.41        | 1.33     |
| 10  | C32   | 1498 | GLY  | C-N   | 5.68  | 1.41        | 1.33     |
| 2   | M     | 415  | ASP  | C-N   | -5.68 | 1.26        | 1.33     |
| 2   | M     | 817  | GLU  | C-N   | -5.67 | 1.26        | 1.34     |
| 22  | I24   | 148  | VAL  | C-N   | 5.67  | 1.42        | 1.33     |
| 10  | C8    | 1342 | SER  | C-N   | -5.67 | 1.26        | 1.33     |
| 18  | B     | 349  | PHE  | C-N   | -5.67 | 1.26        | 1.33     |
| 10  | C32   | 656  | THR  | C-N   | -5.67 | 1.26        | 1.33     |
| 9   | K     | 862  | SER  | C-N   | -5.67 | 1.26        | 1.33     |
| 13  | V     | 749  | GLU  | C-N   | 5.67  | 1.42        | 1.33     |
| 10  | C     | 726  | GLU  | C-N   | 5.67  | 1.42        | 1.33     |
| 10  | C     | 656  | THR  | C-N   | -5.67 | 1.26        | 1.33     |
| 18  | B     | 1673 | ARG  | C-N   | 5.67  | 1.41        | 1.33     |
| 2   | M16   | 338  | ASN  | C-N   | 5.67  | 1.40        | 1.33     |
| 2   | M16   | 624  | ASP  | C-N   | 5.67  | 1.41        | 1.33     |
| 3   | N16   | 53   | THR  | C-N   | -5.67 | 1.25        | 1.33     |
| 10  | C24   | 1793 | VAL  | C-N   | 5.67  | 1.41        | 1.33     |
| 11  | A40   | 51   | THR  | C-N   | 5.67  | 1.41        | 1.34     |
| 11  | A32   | 324  | ARG  | C-N   | -5.67 | 1.26        | 1.33     |
| 18  | B8    | 1673 | ARG  | C-N   | 5.67  | 1.41        | 1.33     |
| 19  | 4     | 292  | SER  | C-N   | -5.67 | 1.25        | 1.33     |
| 21  | H24   | 319  | GLY  | C-N   | -5.67 | 1.25        | 1.33     |
| 10  | C32   | 1410 | LEU  | C-N   | 5.67  | 1.40        | 1.33     |
| 10  | C16   | 1793 | VAL  | C-N   | 5.66  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 422  | THR  | C-N   | -5.66 | 1.25        | 1.33     |
| 21  | H24   | 209  | GLU  | C-N   | -5.66 | 1.26        | 1.33     |
| 10  | C24   | 1719 | ASP  | C-N   | -5.66 | 1.26        | 1.33     |
| 22  | I8    | 328  | TYR  | C-N   | -5.66 | 1.26        | 1.33     |
| 15  | J     | 712  | GLU  | C-N   | -5.66 | 1.26        | 1.33     |
| 23  | J24   | 605  | LEU  | C-N   | -5.66 | 1.26        | 1.33     |
| 10  | C24   | 1410 | LEU  | C-N   | 5.66  | 1.40        | 1.33     |
| 10  | C     | 1342 | SER  | C-N   | -5.66 | 1.26        | 1.33     |
| 6   | O     | 105  | ASN  | C-N   | -5.66 | 1.26        | 1.34     |
| 11  | A32   | 51   | THR  | C-N   | 5.66  | 1.41        | 1.34     |
| 18  | B     | 594  | PHE  | C-N   | 5.66  | 1.41        | 1.33     |
| 2   | M     | 338  | ASN  | C-N   | 5.66  | 1.40        | 1.33     |
| 2   | M16   | 484  | LEU  | C-N   | -5.66 | 1.26        | 1.33     |
| 2   | M16   | 591  | ASP  | C-N   | 5.66  | 1.42        | 1.33     |
| 11  | A40   | 324  | ARG  | C-N   | -5.66 | 1.26        | 1.33     |
| 10  | C8    | 1511 | VAL  | C-N   | 5.66  | 1.40        | 1.33     |
| 23  | J16   | 605  | LEU  | C-N   | -5.66 | 1.26        | 1.33     |
| 10  | C     | 1393 | SER  | C-N   | 5.65  | 1.41        | 1.33     |
| 10  | C8    | 1441 | TYR  | C-N   | 5.65  | 1.42        | 1.33     |
| 2   | M     | 256  | HIS  | C-N   | -5.65 | 1.25        | 1.33     |
| 2   | M     | 591  | ASP  | C-N   | 5.65  | 1.42        | 1.33     |
| 3   | N16   | 194  | ALA  | C-N   | -5.65 | 1.25        | 1.33     |
| 10  | C16   | 654  | PRO  | N-CD  | -5.65 | 1.39        | 1.47     |
| 11  | A24   | 285  | GLN  | C-N   | -5.65 | 1.26        | 1.33     |
| 2   | M     | 163  | SER  | C-N   | 5.65  | 1.41        | 1.33     |
| 6   | O16   | 105  | ASN  | C-N   | -5.65 | 1.26        | 1.34     |
| 22  | I     | 328  | TYR  | C-N   | -5.65 | 1.26        | 1.33     |
| 3   | N     | 53   | THR  | C-N   | -5.65 | 1.25        | 1.33     |
| 11  | A24   | 51   | THR  | C-N   | 5.65  | 1.41        | 1.34     |
| 10  | C24   | 1197 | GLN  | C-N   | -5.65 | 1.26        | 1.33     |
| 18  | B8    | 374  | ILE  | C-N   | -5.65 | 1.26        | 1.34     |
| 18  | B8    | 1249 | LEU  | C-N   | 5.65  | 1.42        | 1.33     |
| 10  | C32   | 422  | THR  | C-N   | -5.65 | 1.25        | 1.33     |
| 10  | C8    | 750  | TYR  | C-N   | -5.65 | 1.26        | 1.33     |
| 22  | I8    | 180  | GLU  | C-N   | -5.65 | 1.26        | 1.33     |
| 10  | C8    | 422  | THR  | C-N   | -5.64 | 1.25        | 1.33     |
| 18  | B8    | 1074 | LYS  | C-N   | 5.64  | 1.41        | 1.34     |
| 22  | I8    | 148  | VAL  | C-N   | 5.64  | 1.42        | 1.33     |
| 23  | J24   | 709  | LYS  | C-N   | -5.64 | 1.26        | 1.33     |
| 10  | C24   | 327  | ILE  | C-N   | 5.64  | 1.41        | 1.33     |
| 10  | C     | 1197 | GLN  | C-N   | -5.64 | 1.26        | 1.33     |
| 11  | A32   | 285  | GLN  | C-N   | -5.64 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M8    | 751  | GLU  | C-N   | 5.64  | 1.41        | 1.33     |
| 21  | H24   | 357  | LYS  | C-N   | -5.64 | 1.26        | 1.33     |
| 22  | I24   | 180  | GLU  | C-N   | -5.64 | 1.26        | 1.33     |
| 2   | M8    | 591  | ASP  | C-N   | 5.64  | 1.42        | 1.33     |
| 10  | C24   | 1331 | CYS  | C-N   | 5.64  | 1.41        | 1.34     |
| 3   | N8    | 53   | THR  | C-N   | -5.64 | 1.25        | 1.33     |
| 1   | R16   | 1355 | ALA  | C-N   | -5.64 | 1.26        | 1.33     |
| 3   | N16   | 44   | GLY  | C-N   | 5.64  | 1.37        | 1.33     |
| 5   | P16   | 158  | VAL  | C-N   | 5.64  | 1.40        | 1.33     |
| 10  | C16   | 422  | THR  | C-N   | -5.64 | 1.25        | 1.33     |
| 13  | V     | 914  | GLU  | C-N   | -5.64 | 1.26        | 1.33     |
| 10  | C8    | 740  | LEU  | C-N   | 5.64  | 1.41        | 1.33     |
| 10  | C8    | 1179 | THR  | C-N   | -5.64 | 1.26        | 1.33     |
| 22  | I16   | 328  | TYR  | C-N   | -5.64 | 1.26        | 1.33     |
| 9   | K8    | 862  | SER  | C-N   | -5.63 | 1.26        | 1.33     |
| 9   | K8    | 1140 | GLN  | C-N   | 5.63  | 1.41        | 1.33     |
| 10  | C8    | 1084 | LYS  | C-N   | -5.63 | 1.25        | 1.33     |
| 10  | C16   | 1197 | GLN  | C-N   | -5.63 | 1.26        | 1.33     |
| 19  | 48    | 340  | PRO  | N-CD  | 5.63  | 1.55        | 1.47     |
| 10  | C32   | 750  | TYR  | C-N   | -5.63 | 1.26        | 1.33     |
| 18  | B     | 1708 | ARG  | C-N   | -5.63 | 1.26        | 1.33     |
| 3   | N     | 194  | ALA  | C-N   | -5.63 | 1.25        | 1.33     |
| 2   | M16   | 256  | HIS  | C-N   | -5.63 | 1.25        | 1.33     |
| 10  | C16   | 1498 | GLY  | C-N   | 5.63  | 1.41        | 1.33     |
| 14  | W     | 688  | HIS  | C-N   | -5.63 | 1.26        | 1.33     |
| 11  | A16   | 324  | ARG  | C-N   | -5.63 | 1.26        | 1.33     |
| 10  | C32   | 740  | LEU  | C-N   | 5.63  | 1.41        | 1.33     |
| 18  | B     | 1074 | LYS  | C-N   | 5.63  | 1.41        | 1.34     |
| 10  | C     | 1084 | LYS  | C-N   | -5.62 | 1.25        | 1.33     |
| 5   | P8    | 158  | VAL  | C-N   | 5.62  | 1.40        | 1.33     |
| 10  | C16   | 1342 | SER  | C-N   | -5.62 | 1.26        | 1.33     |
| 10  | C24   | 1084 | LYS  | C-N   | -5.62 | 1.25        | 1.33     |
| 13  | V     | 853  | GLN  | C-N   | -5.62 | 1.26        | 1.33     |
| 19  | 4     | 340  | PRO  | N-CD  | 5.62  | 1.55        | 1.47     |
| 10  | C32   | 1342 | SER  | C-N   | -5.62 | 1.26        | 1.33     |
| 2   | M8    | 484  | LEU  | C-N   | -5.62 | 1.26        | 1.33     |
| 10  | C     | 654  | PRO  | N-CD  | -5.62 | 1.39        | 1.47     |
| 10  | C32   | 508  | ILE  | C-N   | -5.62 | 1.26        | 1.33     |
| 9   | K     | 638  | TRP  | C-N   | 5.62  | 1.41        | 1.33     |
| 15  | J     | 577  | GLN  | C-N   | -5.61 | 1.26        | 1.33     |
| 12  | A48   | 285  | GLN  | C-N   | -5.61 | 1.26        | 1.33     |
| 5   | P8    | 412  | GLU  | C-N   | -5.61 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 726  | GLU  | C-N   | 5.61  | 1.42        | 1.33     |
| 10  | C     | 1122 | LEU  | C-N   | 5.61  | 1.41        | 1.33     |
| 10  | C     | 1410 | LEU  | C-N   | 5.61  | 1.40        | 1.33     |
| 2   | M16   | 163  | SER  | C-N   | 5.61  | 1.41        | 1.33     |
| 10  | C8    | 157  | GLY  | C-N   | -5.61 | 1.26        | 1.33     |
| 10  | C8    | 508  | ILE  | C-N   | -5.61 | 1.26        | 1.33     |
| 10  | C8    | 1410 | LEU  | C-N   | 5.61  | 1.40        | 1.33     |
| 11  | A16   | 51   | THR  | C-N   | 5.61  | 1.41        | 1.34     |
| 18  | B     | 961  | PRO  | C-N   | 5.61  | 1.41        | 1.33     |
| 3   | N8    | 194  | ALA  | C-N   | -5.61 | 1.25        | 1.33     |
| 1   | R16   | 1259 | ASN  | C-N   | 5.61  | 1.40        | 1.33     |
| 10  | C24   | 157  | GLY  | C-N   | -5.61 | 1.26        | 1.33     |
| 14  | W     | 638  | VAL  | C-N   | -5.61 | 1.26        | 1.33     |
| 21  | H     | 319  | GLY  | C-N   | -5.61 | 1.25        | 1.33     |
| 10  | C32   | 654  | PRO  | N-CD  | -5.61 | 1.39        | 1.47     |
| 10  | C16   | 1380 | GLU  | C-N   | -5.61 | 1.26        | 1.33     |
| 10  | C     | 1179 | THR  | C-N   | -5.61 | 1.26        | 1.33     |
| 18  | B     | 1366 | LYS  | C-N   | -5.61 | 1.27        | 1.33     |
| 18  | B8    | 181  | SER  | C-N   | -5.61 | 1.26        | 1.33     |
| 10  | C32   | 1393 | SER  | C-N   | 5.61  | 1.41        | 1.33     |
| 9   | K     | 619  | GLU  | C-N   | -5.60 | 1.25        | 1.33     |
| 9   | K     | 629  | SER  | C-N   | -5.60 | 1.26        | 1.33     |
| 10  | C24   | 1393 | SER  | C-N   | 5.60  | 1.41        | 1.33     |
| 12  | A     | 324  | ARG  | C-N   | -5.60 | 1.26        | 1.33     |
| 18  | B8    | 1708 | ARG  | C-N   | -5.60 | 1.26        | 1.33     |
| 21  | H8    | 319  | GLY  | C-N   | -5.60 | 1.25        | 1.33     |
| 2   | M     | 751  | GLU  | C-N   | 5.60  | 1.41        | 1.33     |
| 11  | A24   | 713  | ASP  | C-N   | -5.60 | 1.26        | 1.33     |
| 11  | A40   | 285  | GLN  | C-N   | -5.60 | 1.26        | 1.33     |
| 10  | C8    | 654  | PRO  | N-CD  | -5.60 | 1.40        | 1.47     |
| 18  | B8    | 821  | PHE  | C-N   | 5.60  | 1.40        | 1.33     |
| 21  | H     | 209  | GLU  | C-N   | -5.60 | 1.26        | 1.33     |
| 10  | C     | 1380 | GLU  | C-N   | -5.60 | 1.26        | 1.33     |
| 17  | F24   | 76   | ASP  | C-N   | 5.60  | 1.42        | 1.33     |
| 20  | E     | 90   | SER  | C-N   | -5.60 | 1.23        | 1.33     |
| 12  | A48   | 713  | ASP  | C-N   | -5.60 | 1.26        | 1.33     |
| 6   | O16   | 152  | GLU  | C-N   | -5.59 | 1.26        | 1.33     |
| 9   | K     | 1135 | THR  | C-N   | -5.59 | 1.26        | 1.34     |
| 9   | K8    | 619  | GLU  | C-N   | -5.59 | 1.25        | 1.33     |
| 9   | K8    | 1135 | THR  | C-N   | -5.59 | 1.26        | 1.34     |
| 10  | C8    | 770  | SER  | C-N   | 5.59  | 1.41        | 1.33     |
| 20  | E     | 498  | LYS  | C-N   | -5.59 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 637  | HIS  | C-N   | -5.59 | 1.25        | 1.33     |
| 11  | A24   | 324  | ARG  | C-N   | -5.59 | 1.26        | 1.33     |
| 10  | C8    | 1498 | GLY  | C-N   | 5.59  | 1.41        | 1.33     |
| 19  | 48    | 249  | PRO  | C-N   | -5.59 | 1.26        | 1.33     |
| 12  | A     | 713  | ASP  | C-N   | -5.59 | 1.26        | 1.33     |
| 10  | C32   | 1340 | PRO  | C-N   | -5.59 | 1.26        | 1.34     |
| 10  | C24   | 1498 | GLY  | C-N   | 5.59  | 1.41        | 1.33     |
| 10  | C     | 1339 | VAL  | C-N   | -5.59 | 1.26        | 1.33     |
| 5   | P8    | 641  | GLN  | C-N   | -5.59 | 1.26        | 1.33     |
| 10  | C16   | 750  | TYR  | C-N   | -5.59 | 1.26        | 1.33     |
| 12  | A     | 431  | ARG  | C-N   | -5.59 | 1.26        | 1.33     |
| 15  | J     | 605  | LEU  | C-N   | -5.59 | 1.26        | 1.33     |
| 10  | C     | 1511 | VAL  | C-N   | 5.59  | 1.40        | 1.33     |
| 19  | 48    | 4    | PHE  | C-N   | -5.59 | 1.27        | 1.33     |
| 1   | R8    | 1259 | ASN  | C-N   | 5.58  | 1.40        | 1.33     |
| 18  | B     | 15   | PRO  | C-N   | -5.58 | 1.25        | 1.33     |
| 24  | D     | 1440 | PRO  | CA-C  | 5.58  | 1.54        | 1.51     |
| 1   | R8    | 1355 | ALA  | C-N   | -5.58 | 1.26        | 1.33     |
| 9   | K     | 753  | ASP  | C-N   | 5.58  | 1.41        | 1.33     |
| 10  | C16   | 149  | PRO  | C-N   | 5.58  | 1.41        | 1.33     |
| 10  | C     | 149  | PRO  | C-N   | 5.58  | 1.41        | 1.33     |
| 9   | K8    | 638  | TRP  | C-N   | 5.58  | 1.41        | 1.33     |
| 20  | E8    | 90   | SER  | C-N   | -5.58 | 1.23        | 1.33     |
| 21  | H8    | 209  | GLU  | C-N   | -5.58 | 1.26        | 1.33     |
| 9   | K8    | 753  | ASP  | C-N   | 5.58  | 1.41        | 1.33     |
| 9   | K8    | 844  | SER  | C-N   | -5.58 | 1.26        | 1.33     |
| 10  | C     | 1498 | GLY  | C-N   | 5.58  | 1.41        | 1.33     |
| 10  | C8    | 149  | PRO  | C-N   | 5.58  | 1.41        | 1.33     |
| 19  | 4     | 4    | PHE  | C-N   | -5.58 | 1.27        | 1.33     |
| 23  | J8    | 605  | LEU  | C-N   | -5.58 | 1.26        | 1.33     |
| 5   | P     | 641  | GLN  | C-N   | -5.58 | 1.26        | 1.33     |
| 10  | C8    | 1122 | LEU  | C-N   | 5.58  | 1.41        | 1.33     |
| 5   | P     | 158  | VAL  | C-N   | 5.58  | 1.40        | 1.33     |
| 10  | C24   | 1340 | PRO  | C-N   | -5.58 | 1.26        | 1.34     |
| 10  | C24   | 1342 | SER  | C-N   | -5.58 | 1.26        | 1.33     |
| 18  | B8    | 961  | PRO  | C-N   | 5.58  | 1.41        | 1.33     |
| 22  | I8    | 297  | HIS  | C-N   | 5.58  | 1.41        | 1.33     |
| 13  | V     | 829  | ARG  | C-N   | -5.57 | 1.26        | 1.33     |
| 10  | C     | 1328 | PHE  | C-N   | -5.57 | 1.26        | 1.33     |
| 18  | B8    | 933  | GLN  | C-N   | -5.57 | 1.26        | 1.33     |
| 19  | 48    | 385  | TYR  | C-N   | -5.57 | 1.25        | 1.33     |
| 24  | D8    | 1440 | PRO  | CA-C  | 5.57  | 1.54        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M16   | 751  | GLU  | C-N   | 5.57  | 1.41        | 1.33     |
| 20  | E8    | 498  | LYS  | C-N   | -5.57 | 1.27        | 1.33     |
| 23  | J32   | 605  | LEU  | C-N   | -5.57 | 1.26        | 1.33     |
| 2   | M16   | 605  | SER  | C-N   | 5.57  | 1.41        | 1.33     |
| 9   | K8    | 763  | LYS  | C-N   | -5.57 | 1.26        | 1.33     |
| 10  | C16   | 1179 | THR  | C-N   | -5.57 | 1.26        | 1.33     |
| 21  | H8    | 274  | THR  | C-N   | -5.57 | 1.26        | 1.33     |
| 22  | I24   | 328  | TYR  | C-N   | -5.57 | 1.26        | 1.33     |
| 18  | B8    | 1619 | ILE  | C-N   | 5.57  | 1.41        | 1.33     |
| 5   | P     | 412  | GLU  | C-N   | -5.57 | 1.26        | 1.33     |
| 6   | O16   | 158  | ASP  | C-N   | 5.57  | 1.41        | 1.33     |
| 11  | A40   | 582  | ASP  | C-N   | 5.57  | 1.41        | 1.34     |
| 10  | C     | 268  | ILE  | C-N   | -5.57 | 1.26        | 1.33     |
| 11  | A16   | 285  | GLN  | C-N   | -5.57 | 1.26        | 1.33     |
| 17  | F8    | 76   | ASP  | C-N   | 5.57  | 1.42        | 1.33     |
| 10  | C32   | 1179 | THR  | C-N   | -5.57 | 1.26        | 1.33     |
| 12  | A48   | 324  | ARG  | C-N   | -5.57 | 1.26        | 1.33     |
| 1   | R     | 1351 | PRO  | N-CD  | 5.57  | 1.55        | 1.47     |
| 5   | P8    | 287  | MET  | C-N   | 5.57  | 1.39        | 1.33     |
| 5   | P16   | 641  | GLN  | C-N   | -5.57 | 1.26        | 1.33     |
| 10  | C24   | 740  | LEU  | C-N   | 5.57  | 1.41        | 1.33     |
| 10  | C24   | 804  | PRO  | C-N   | -5.57 | 1.26        | 1.33     |
| 18  | B     | 398  | ILE  | C-N   | -5.57 | 1.26        | 1.33     |
| 20  | E     | 177  | SER  | C-N   | -5.57 | 1.26        | 1.33     |
| 2   | M8    | 605  | SER  | C-N   | 5.56  | 1.41        | 1.33     |
| 21  | H24   | 274  | THR  | C-N   | -5.56 | 1.26        | 1.33     |
| 9   | K8    | 637  | HIS  | C-N   | -5.56 | 1.25        | 1.33     |
| 9   | K8    | 748  | THR  | C-N   | -5.56 | 1.27        | 1.34     |
| 10  | C16   | 740  | LEU  | C-N   | 5.56  | 1.41        | 1.33     |
| 10  | C8    | 1339 | VAL  | C-N   | -5.56 | 1.26        | 1.33     |
| 19  | 4     | 249  | PRO  | C-N   | -5.56 | 1.26        | 1.33     |
| 10  | C16   | 508  | ILE  | C-N   | -5.56 | 1.26        | 1.33     |
| 3   | N8    | 44   | GLY  | C-N   | 5.56  | 1.37        | 1.33     |
| 11  | A40   | 810  | PRO  | C-N   | -5.56 | 1.26        | 1.34     |
| 10  | C8    | 609  | SER  | C-N   | -5.56 | 1.26        | 1.33     |
| 20  | E     | 503  | THR  | C-N   | -5.56 | 1.26        | 1.34     |
| 12  | A48   | 111  | MET  | C-N   | -5.56 | 1.26        | 1.33     |
| 5   | P8    | 698  | GLY  | C-N   | -5.56 | 1.26        | 1.33     |
| 10  | C     | 508  | ILE  | C-N   | -5.56 | 1.26        | 1.33     |
| 18  | B8    | 594  | PHE  | C-N   | 5.56  | 1.41        | 1.33     |
| 10  | C     | 1340 | PRO  | C-N   | -5.56 | 1.26        | 1.34     |
| 6   | O16   | 108  | SER  | C-N   | 5.55  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A24   | 111  | MET  | C-N   | -5.55 | 1.26        | 1.33     |
| 10  | C24   | 750  | TYR  | C-N   | -5.55 | 1.26        | 1.33     |
| 11  | A40   | 431  | ARG  | C-N   | -5.55 | 1.26        | 1.33     |
| 10  | C32   | 3    | SER  | C-N   | -5.55 | 1.25        | 1.33     |
| 12  | A     | 111  | MET  | C-N   | -5.55 | 1.26        | 1.33     |
| 10  | C     | 1392 | ALA  | C-N   | 5.55  | 1.41        | 1.33     |
| 21  | H     | 274  | THR  | C-N   | -5.55 | 1.26        | 1.33     |
| 10  | C32   | 1511 | VAL  | C-N   | 5.55  | 1.40        | 1.33     |
| 1   | R     | 1259 | ASN  | C-N   | 5.55  | 1.40        | 1.33     |
| 10  | C24   | 1179 | THR  | C-N   | -5.55 | 1.26        | 1.33     |
| 10  | C8    | 1380 | GLU  | C-N   | -5.55 | 1.26        | 1.33     |
| 17  | F     | 76   | ASP  | C-N   | 5.55  | 1.42        | 1.33     |
| 20  | E8    | 177  | SER  | C-N   | -5.55 | 1.26        | 1.33     |
| 2   | M16   | 459  | LEU  | C-N   | 5.55  | 1.41        | 1.33     |
| 10  | C8    | 3    | SER  | C-N   | -5.55 | 1.25        | 1.33     |
| 10  | C8    | 1338 | ASP  | C-N   | 5.55  | 1.38        | 1.33     |
| 18  | B     | 374  | ILE  | C-N   | -5.55 | 1.26        | 1.34     |
| 20  | E8    | 350  | GLU  | C-N   | -5.55 | 1.25        | 1.33     |
| 22  | I24   | 297  | HIS  | C-N   | 5.55  | 1.41        | 1.33     |
| 10  | C16   | 1340 | PRO  | C-N   | -5.55 | 1.26        | 1.34     |
| 10  | C     | 740  | LEU  | C-N   | 5.55  | 1.41        | 1.33     |
| 9   | K     | 748  | THR  | C-N   | -5.54 | 1.27        | 1.34     |
| 18  | B8    | 654  | CYS  | C-N   | 5.54  | 1.41        | 1.33     |
| 2   | M8    | 211  | MET  | C-N   | 5.54  | 1.40        | 1.33     |
| 9   | K     | 960  | LYS  | C-N   | -5.54 | 1.26        | 1.33     |
| 9   | K     | 1140 | GLN  | C-N   | 5.54  | 1.41        | 1.33     |
| 10  | C24   | 1380 | GLU  | C-N   | -5.54 | 1.26        | 1.33     |
| 22  | I     | 297  | HIS  | C-N   | 5.54  | 1.41        | 1.33     |
| 2   | M16   | 488  | HIS  | C-N   | -5.54 | 1.26        | 1.33     |
| 1   | R     | 1355 | ALA  | C-N   | -5.54 | 1.26        | 1.33     |
| 5   | P16   | 698  | GLY  | C-N   | -5.54 | 1.26        | 1.33     |
| 11  | A24   | 582  | ASP  | C-N   | 5.54  | 1.41        | 1.34     |
| 11  | A16   | 582  | ASP  | C-N   | 5.54  | 1.41        | 1.34     |
| 18  | B8    | 286  | GLN  | C-N   | -5.54 | 1.26        | 1.33     |
| 18  | B8    | 1062 | SER  | C-N   | 5.54  | 1.41        | 1.33     |
| 20  | E     | 350  | GLU  | C-N   | -5.54 | 1.25        | 1.33     |
| 10  | C     | 1757 | GLN  | C-N   | -5.54 | 1.26        | 1.33     |
| 10  | C8    | 1757 | GLN  | C-N   | -5.54 | 1.26        | 1.33     |
| 1   | R8    | 1351 | PRO  | N-CD  | 5.54  | 1.55        | 1.47     |
| 5   | P     | 12   | GLU  | C-N   | -5.54 | 1.25        | 1.33     |
| 6   | O8    | 158  | ASP  | C-N   | 5.54  | 1.41        | 1.33     |
| 10  | C16   | 1    | MET  | C-N   | -5.54 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C     | 1338 | ASP  | C-N   | 5.54  | 1.38        | 1.33     |
| 11  | A32   | 582  | ASP  | C-N   | 5.54  | 1.41        | 1.34     |
| 10  | C32   | 1139 | ARG  | C-N   | -5.53 | 1.25        | 1.33     |
| 19  | 4     | 385  | TYR  | C-N   | -5.53 | 1.25        | 1.33     |
| 11  | A24   | 431  | ARG  | C-N   | -5.53 | 1.26        | 1.33     |
| 18  | B8    | 398  | ILE  | C-N   | -5.53 | 1.26        | 1.33     |
| 21  | H16   | 274  | THR  | C-N   | -5.53 | 1.26        | 1.33     |
| 6   | O     | 152  | GLU  | C-N   | -5.53 | 1.26        | 1.33     |
| 5   | P16   | 555  | GLU  | C-N   | -5.53 | 1.26        | 1.33     |
| 2   | M     | 211  | MET  | C-N   | 5.53  | 1.40        | 1.33     |
| 10  | C16   | 1139 | ARG  | C-N   | -5.53 | 1.25        | 1.33     |
| 10  | C24   | 508  | ILE  | C-N   | -5.53 | 1.26        | 1.33     |
| 13  | V     | 759  | ALA  | C-N   | 5.53  | 1.41        | 1.33     |
| 17  | F16   | 76   | ASP  | C-N   | 5.53  | 1.42        | 1.33     |
| 18  | B     | 1379 | VAL  | C-N   | 5.53  | 1.41        | 1.33     |
| 18  | B     | 1938 | LYS  | C-N   | -5.53 | 1.26        | 1.34     |
| 2   | M8    | 516  | VAL  | C-N   | -5.53 | 1.26        | 1.33     |
| 12  | A     | 582  | ASP  | C-N   | 5.53  | 1.41        | 1.34     |
| 22  | I16   | 297  | HIS  | C-N   | 5.53  | 1.41        | 1.33     |
| 24  | D40   | 1440 | PRO  | CA-C  | 5.53  | 1.54        | 1.51     |
| 18  | B8    | 1394 | TRP  | C-N   | 5.52  | 1.42        | 1.33     |
| 9   | K8    | 629  | SER  | C-N   | -5.52 | 1.26        | 1.33     |
| 12  | A     | 432  | GLN  | C-N   | -5.52 | 1.26        | 1.33     |
| 10  | C32   | 1    | MET  | C-N   | -5.52 | 1.26        | 1.33     |
| 10  | C32   | 157  | GLY  | C-N   | -5.52 | 1.26        | 1.33     |
| 2   | M     | 484  | LEU  | C-N   | -5.52 | 1.26        | 1.33     |
| 9   | K8    | 1123 | ARG  | C-N   | 5.52  | 1.41        | 1.33     |
| 10  | C8    | 1139 | ARG  | C-N   | -5.52 | 1.25        | 1.33     |
| 19  | 4     | 445  | VAL  | C-N   | -5.52 | 1.24        | 1.33     |
| 20  | E8    | 93   | GLU  | C-N   | -5.52 | 1.26        | 1.33     |
| 10  | C32   | 804  | PRO  | C-N   | -5.52 | 1.26        | 1.33     |
| 2   | M8    | 163  | SER  | C-N   | 5.52  | 1.41        | 1.33     |
| 1   | R16   | 1252 | VAL  | C-N   | -5.52 | 1.26        | 1.33     |
| 7   | Q     | 239  | ARG  | C-N   | -5.52 | 1.25        | 1.33     |
| 10  | C16   | 1122 | LEU  | C-N   | 5.52  | 1.41        | 1.33     |
| 10  | C8    | 1328 | PHE  | C-N   | -5.52 | 1.26        | 1.33     |
| 19  | 48    | 445  | VAL  | C-N   | -5.52 | 1.24        | 1.33     |
| 10  | C24   | 1    | MET  | C-N   | -5.52 | 1.26        | 1.33     |
| 10  | C16   | 3    | SER  | C-N   | -5.51 | 1.25        | 1.33     |
| 18  | B8    | 1604 | ASN  | C-N   | 5.51  | 1.41        | 1.33     |
| 9   | K     | 844  | SER  | C-N   | -5.51 | 1.26        | 1.33     |
| 10  | C16   | 804  | PRO  | C-N   | -5.51 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 1139 | ARG  | C-N   | -5.51 | 1.25        | 1.33     |
| 18  | B8    | 1318 | ALA  | C-N   | 5.51  | 1.41        | 1.33     |
| 10  | C32   | 1380 | GLU  | C-N   | -5.51 | 1.26        | 1.33     |
| 11  | A32   | 803  | PRO  | N-CD  | -5.51 | 1.40        | 1.47     |
| 18  | B     | 654  | CYS  | C-N   | 5.51  | 1.41        | 1.33     |
| 10  | C16   | 1338 | ASP  | C-N   | 5.51  | 1.38        | 1.33     |
| 10  | C     | 1139 | ARG  | C-N   | -5.51 | 1.25        | 1.33     |
| 21  | H     | 354  | ASN  | C-N   | -5.51 | 1.26        | 1.33     |
| 2   | M     | 605  | SER  | C-N   | 5.51  | 1.41        | 1.33     |
| 3   | N8    | 210  | THR  | C-N   | -5.51 | 1.26        | 1.33     |
| 5   | P8    | 151  | LEU  | C-N   | 5.51  | 1.41        | 1.33     |
| 14  | W     | 650  | LYS  | C-N   | -5.51 | 1.26        | 1.33     |
| 10  | C     | 770  | SER  | C-N   | 5.51  | 1.41        | 1.33     |
| 11  | A24   | 803  | PRO  | N-CD  | -5.50 | 1.40        | 1.47     |
| 6   | O     | 222  | PRO  | N-CD  | 5.50  | 1.55        | 1.47     |
| 5   | P16   | 572  | SER  | C-N   | 5.50  | 1.41        | 1.33     |
| 10  | C24   | 268  | ILE  | C-N   | -5.50 | 1.26        | 1.33     |
| 21  | H16   | 163  | PRO  | N-CD  | -5.50 | 1.40        | 1.47     |
| 21  | H16   | 209  | GLU  | C-N   | -5.50 | 1.26        | 1.33     |
| 6   | O     | 158  | ASP  | C-N   | 5.50  | 1.41        | 1.33     |
| 18  | B8    | 15   | PRO  | C-N   | -5.50 | 1.25        | 1.33     |
| 10  | C16   | 1750 | GLN  | C-N   | -5.50 | 1.26        | 1.33     |
| 18  | B     | 933  | GLN  | C-N   | -5.50 | 1.26        | 1.33     |
| 18  | B8    | 1938 | LYS  | C-N   | -5.50 | 1.26        | 1.34     |
| 12  | A48   | 582  | ASP  | C-N   | 5.50  | 1.41        | 1.34     |
| 2   | M     | 516  | VAL  | C-N   | -5.50 | 1.26        | 1.33     |
| 6   | O     | 108  | SER  | C-N   | 5.50  | 1.41        | 1.33     |
| 11  | A40   | 432  | GLN  | C-N   | -5.50 | 1.26        | 1.33     |
| 11  | A40   | 781  | LEU  | C-N   | -5.50 | 1.27        | 1.33     |
| 14  | W     | 754  | VAL  | C-N   | 5.50  | 1.40        | 1.33     |
| 15  | J     | 593  | VAL  | C-N   | -5.50 | 1.26        | 1.33     |
| 16  | A8    | 111  | MET  | C-N   | -5.50 | 1.26        | 1.33     |
| 18  | B     | 1633 | SER  | C-N   | 5.50  | 1.41        | 1.33     |
| 18  | B8    | 40   | LEU  | C-N   | 5.50  | 1.41        | 1.34     |
| 11  | A32   | 810  | PRO  | C-N   | -5.50 | 1.26        | 1.34     |
| 2   | M8    | 488  | HIS  | C-N   | -5.49 | 1.26        | 1.33     |
| 5   | P     | 151  | LEU  | C-N   | 5.49  | 1.41        | 1.33     |
| 5   | P16   | 622  | ALA  | C-N   | -5.49 | 1.26        | 1.33     |
| 10  | C     | 157  | GLY  | C-N   | -5.49 | 1.26        | 1.33     |
| 6   | O8    | 152  | GLU  | C-N   | -5.49 | 1.26        | 1.33     |
| 7   | Q8    | 208  | ARG  | C-N   | -5.49 | 1.25        | 1.33     |
| 10  | C16   | 157  | GLY  | C-N   | -5.49 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | C24   | 149  | PRO  | C-N     | 5.49  | 1.41        | 1.33     |
| 10  | C24   | 1122 | LEU  | C-N     | 5.49  | 1.41        | 1.33     |
| 10  | C32   | 1392 | ALA  | C-N     | 5.49  | 1.41        | 1.33     |
| 5   | P     | 572  | SER  | C-N     | 5.49  | 1.41        | 1.33     |
| 5   | P     | 709  | GLY  | C-N     | -5.49 | 1.26        | 1.33     |
| 9   | K     | 1204 | THR  | C-N     | 5.49  | 1.41        | 1.34     |
| 10  | C     | 233  | ASP  | C-N     | -5.49 | 1.27        | 1.33     |
| 10  | C8    | 1    | MET  | C-N     | -5.49 | 1.27        | 1.33     |
| 5   | P16   | 12   | GLU  | C-N     | -5.49 | 1.26        | 1.33     |
| 10  | C     | 1042 | GLU  | C-N     | -5.49 | 1.26        | 1.33     |
| 11  | A32   | 149  | GLN  | C-N     | -5.49 | 1.26        | 1.34     |
| 7   | Q     | 208  | ARG  | C-N     | -5.49 | 1.25        | 1.33     |
| 10  | C24   | 3    | SER  | C-N     | -5.49 | 1.25        | 1.33     |
| 11  | A40   | 803  | PRO  | N-CD    | -5.49 | 1.40        | 1.47     |
| 12  | A48   | 432  | GLN  | C-N     | -5.49 | 1.27        | 1.33     |
| 12  | A48   | 803  | PRO  | N-CD    | -5.49 | 1.40        | 1.47     |
| 10  | C8    | 804  | PRO  | C-N     | -5.48 | 1.26        | 1.33     |
| 9   | K     | 1123 | ARG  | C-N     | 5.48  | 1.41        | 1.33     |
| 10  | C     | 804  | PRO  | C-N     | -5.48 | 1.26        | 1.33     |
| 10  | C8    | 1340 | PRO  | C-N     | -5.48 | 1.26        | 1.34     |
| 10  | C8    | 1392 | ALA  | C-N     | 5.48  | 1.41        | 1.33     |
| 18  | B     | 1318 | ALA  | C-N     | 5.48  | 1.41        | 1.33     |
| 19  | 4     | 425  | LEU  | C-N     | -5.48 | 1.25        | 1.33     |
| 11  | A16   | 149  | GLN  | C-N     | -5.48 | 1.26        | 1.34     |
| 2   | M     | 488  | HIS  | C-N     | -5.48 | 1.26        | 1.33     |
| 5   | P     | 698  | GLY  | C-N     | -5.48 | 1.26        | 1.33     |
| 5   | P16   | 287  | MET  | C-N     | 5.48  | 1.38        | 1.33     |
| 9   | K     | 763  | LYS  | C-N     | -5.48 | 1.27        | 1.33     |
| 10  | C16   | 233  | ASP  | C-N     | -5.48 | 1.27        | 1.33     |
| 10  | C8    | 268  | ILE  | C-N     | -5.48 | 1.26        | 1.33     |
| 18  | B8    | 278  | THR  | C-N     | 5.48  | 1.41        | 1.33     |
| 12  | A48   | 431  | ARG  | C-N     | -5.48 | 1.26        | 1.33     |
| 5   | P16   | 151  | LEU  | C-N     | 5.48  | 1.40        | 1.33     |
| 10  | C16   | 268  | ILE  | C-N     | -5.48 | 1.26        | 1.33     |
| 11  | A32   | 406  | MET  | C-N     | -5.48 | 1.26        | 1.33     |
| 18  | B8    | 650  | LYS  | C-N     | 5.47  | 1.41        | 1.33     |
| 19  | 4     | 330  | LYS  | C-N     | -5.47 | 1.26        | 1.33     |
| 22  | I16   | 209  | TRP  | NE1-CE2 | -5.47 | 1.31        | 1.37     |
| 1   | R     | 1258 | ALA  | C-N     | 5.47  | 1.41        | 1.33     |
| 1   | R16   | 1351 | PRO  | N-CD    | 5.47  | 1.55        | 1.47     |
| 10  | C24   | 609  | SER  | C-N     | -5.47 | 1.26        | 1.33     |
| 12  | A     | 447  | ILE  | C-N     | -5.47 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | A     | 803  | PRO  | N-CD    | -5.47 | 1.40        | 1.47     |
| 1   | R     | 1440 | PRO  | C-N     | -5.47 | 1.26        | 1.34     |
| 5   | P8    | 12   | GLU  | C-N     | -5.47 | 1.26        | 1.33     |
| 7   | Q16   | 208  | ARG  | C-N     | -5.47 | 1.25        | 1.33     |
| 10  | C     | 3    | SER  | C-N     | -5.47 | 1.25        | 1.33     |
| 18  | B8    | 817  | CYS  | C-N     | 5.47  | 1.42        | 1.33     |
| 10  | C     | 1154 | TRP  | NE1-CE2 | -5.47 | 1.31        | 1.37     |
| 5   | P8    | 709  | GLY  | C-N     | -5.47 | 1.26        | 1.33     |
| 15  | J     | 611  | GLN  | C-N     | -5.47 | 1.26        | 1.33     |
| 10  | C8    | 233  | ASP  | C-N     | -5.47 | 1.27        | 1.33     |
| 2   | M8    | 459  | LEU  | C-N     | 5.47  | 1.41        | 1.33     |
| 9   | K8    | 960  | LYS  | C-N     | -5.47 | 1.26        | 1.33     |
| 10  | C8    | 1750 | GLN  | C-N     | -5.47 | 1.26        | 1.33     |
| 21  | H8    | 354  | ASN  | C-N     | -5.47 | 1.27        | 1.33     |
| 1   | R8    | 1252 | VAL  | C-N     | -5.46 | 1.26        | 1.33     |
| 7   | Q8    | 239  | ARG  | C-N     | -5.46 | 1.25        | 1.33     |
| 9   | K8    | 858  | ILE  | C-N     | -5.46 | 1.26        | 1.33     |
| 18  | B     | 232  | GLU  | C-N     | -5.46 | 1.26        | 1.33     |
| 20  | E     | 93   | GLU  | C-N     | -5.46 | 1.26        | 1.33     |
| 20  | E8    | 503  | THR  | C-N     | -5.46 | 1.26        | 1.34     |
| 21  | H24   | 354  | ASN  | C-N     | -5.46 | 1.27        | 1.33     |
| 5   | P     | 555  | GLU  | C-N     | -5.46 | 1.26        | 1.33     |
| 18  | B8    | 1633 | SER  | C-N     | 5.46  | 1.41        | 1.33     |
| 22  | I8    | 209  | TRP  | NE1-CE2 | -5.46 | 1.31        | 1.37     |
| 10  | C8    | 1042 | GLU  | C-N     | -5.46 | 1.26        | 1.33     |
| 18  | B     | 278  | THR  | C-N     | 5.46  | 1.41        | 1.33     |
| 18  | B     | 286  | GLN  | C-N     | -5.46 | 1.26        | 1.33     |
| 19  | 48    | 330  | LYS  | C-N     | -5.46 | 1.26        | 1.33     |
| 21  | H     | 163  | PRO  | N-CD    | -5.46 | 1.40        | 1.47     |
| 9   | K     | 869  | GLU  | C-N     | -5.46 | 1.27        | 1.33     |
| 10  | C16   | 1392 | ALA  | C-N     | 5.46  | 1.41        | 1.33     |
| 5   | P16   | 210  | ILE  | C-N     | -5.46 | 1.26        | 1.33     |
| 10  | C24   | 1392 | ALA  | C-N     | 5.46  | 1.41        | 1.33     |
| 10  | C32   | 1042 | GLU  | C-N     | -5.46 | 1.26        | 1.33     |
| 14  | W     | 630  | ASN  | C-N     | -5.46 | 1.25        | 1.33     |
| 18  | B     | 363  | PHE  | C-N     | 5.46  | 1.41        | 1.33     |
| 18  | B     | 1394 | TRP  | C-N     | 5.46  | 1.42        | 1.33     |
| 18  | B     | 1604 | ASN  | C-N     | 5.46  | 1.41        | 1.33     |
| 20  | E     | 120  | ALA  | C-N     | -5.46 | 1.27        | 1.33     |
| 10  | C32   | 609  | SER  | C-N     | -5.46 | 1.27        | 1.33     |
| 2   | M16   | 211  | MET  | C-N     | 5.46  | 1.40        | 1.33     |
| 5   | P8    | 210  | ILE  | C-N     | -5.46 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C     | 1    | MET  | C-N   | -5.46 | 1.27        | 1.33     |
| 6   | O8    | 225  | LYS  | C-N   | -5.45 | 1.25        | 1.33     |
| 10  | C     | 609  | SER  | C-N   | -5.45 | 1.27        | 1.33     |
| 18  | B8    | 1667 | ASP  | C-N   | 5.45  | 1.45        | 1.33     |
| 20  | E     | 180  | THR  | C-N   | -5.45 | 1.26        | 1.33     |
| 10  | C32   | 149  | PRO  | C-N   | 5.45  | 1.41        | 1.33     |
| 10  | C32   | 1750 | GLN  | C-N   | -5.45 | 1.26        | 1.33     |
| 6   | O8    | 222  | PRO  | N-CD  | 5.45  | 1.55        | 1.47     |
| 10  | C8    | 505  | PHE  | C-N   | -5.45 | 1.26        | 1.33     |
| 18  | B     | 821  | PHE  | C-N   | 5.45  | 1.40        | 1.33     |
| 18  | B     | 1062 | SER  | C-N   | 5.45  | 1.41        | 1.33     |
| 3   | N     | 210  | THR  | C-N   | -5.45 | 1.26        | 1.33     |
| 10  | C     | 563  | THR  | C-N   | -5.45 | 1.25        | 1.33     |
| 10  | C32   | 1424 | GLN  | C-N   | 5.45  | 1.41        | 1.34     |
| 21  | H24   | 163  | PRO  | N-CD  | -5.45 | 1.40        | 1.47     |
| 10  | C32   | 233  | ASP  | C-N   | -5.45 | 1.27        | 1.33     |
| 10  | C24   | 1750 | GLN  | C-N   | -5.45 | 1.26        | 1.33     |
| 18  | B8    | 566  | LYS  | C-N   | -5.45 | 1.26        | 1.34     |
| 5   | P8    | 397  | HIS  | C-N   | -5.45 | 1.26        | 1.33     |
| 5   | P8    | 622  | ALA  | C-N   | -5.45 | 1.26        | 1.33     |
| 18  | B8    | 1201 | LYS  | C-N   | -5.45 | 1.27        | 1.33     |
| 10  | C     | 1750 | GLN  | C-N   | -5.44 | 1.26        | 1.33     |
| 5   | P16   | 709  | GLY  | C-N   | -5.44 | 1.26        | 1.33     |
| 9   | K8    | 869  | GLU  | C-N   | -5.44 | 1.27        | 1.33     |
| 10  | C16   | 1042 | GLU  | C-N   | -5.44 | 1.26        | 1.33     |
| 18  | B8    | 1724 | MET  | C-N   | -5.44 | 1.26        | 1.33     |
| 18  | B     | 650  | LYS  | C-N   | 5.44  | 1.41        | 1.33     |
| 18  | B     | 1201 | LYS  | C-N   | -5.44 | 1.27        | 1.33     |
| 20  | E8    | 460  | ALA  | C-N   | -5.44 | 1.26        | 1.33     |
| 2   | M8    | 487  | TRP  | C-N   | 5.44  | 1.42        | 1.33     |
| 9   | K8    | 1234 | ARG  | C-N   | -5.44 | 1.26        | 1.33     |
| 10  | C32   | 268  | ILE  | C-N   | -5.44 | 1.27        | 1.33     |
| 5   | P     | 210  | ILE  | C-N   | -5.44 | 1.26        | 1.33     |
| 5   | P     | 397  | HIS  | C-N   | -5.44 | 1.26        | 1.33     |
| 5   | P8    | 583  | GLY  | C-N   | -5.44 | 1.26        | 1.33     |
| 6   | O8    | 108  | SER  | C-N   | 5.44  | 1.41        | 1.33     |
| 10  | C24   | 875  | LEU  | C-N   | -5.44 | 1.26        | 1.33     |
| 11  | A40   | 111  | MET  | C-N   | -5.44 | 1.26        | 1.33     |
| 18  | B     | 40   | LEU  | C-N   | 5.44  | 1.41        | 1.34     |
| 18  | B     | 1034 | ALA  | C-N   | 5.44  | 1.41        | 1.33     |
| 18  | B8    | 1802 | ASP  | C-N   | -5.44 | 1.26        | 1.33     |
| 10  | C32   | 1757 | GLN  | C-N   | -5.44 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | R8    | 1258 | ALA  | C-N     | 5.44  | 1.41        | 1.33     |
| 11  | A16   | 803  | PRO  | N-CD    | -5.44 | 1.40        | 1.47     |
| 1   | R     | 1128 | ALA  | C-N     | -5.43 | 1.26        | 1.33     |
| 19  | 48    | 26   | SER  | C-N     | -5.43 | 1.26        | 1.34     |
| 5   | P     | 604  | TYR  | C-N     | -5.43 | 1.26        | 1.33     |
| 6   | O     | 225  | LYS  | C-N     | -5.43 | 1.25        | 1.33     |
| 5   | P16   | 604  | TYR  | C-N     | -5.43 | 1.26        | 1.33     |
| 9   | K     | 1153 | ALA  | C-N     | -5.43 | 1.25        | 1.33     |
| 9   | K     | 1234 | ARG  | C-N     | -5.43 | 1.26        | 1.33     |
| 9   | K8    | 1143 | TRP  | C-N     | -5.43 | 1.26        | 1.34     |
| 10  | C24   | 1042 | GLU  | C-N     | -5.43 | 1.26        | 1.33     |
| 18  | B     | 12   | TRP  | C-N     | 5.43  | 1.40        | 1.33     |
| 10  | C32   | 505  | PHE  | C-N     | -5.43 | 1.26        | 1.33     |
| 5   | P8    | 572  | SER  | C-N     | 5.43  | 1.41        | 1.33     |
| 1   | R8    | 1440 | PRO  | C-N     | -5.43 | 1.26        | 1.34     |
| 8   | L     | 346  | TRP  | NE1-CE2 | -5.43 | 1.31        | 1.37     |
| 11  | A32   | 432  | GLN  | C-N     | -5.43 | 1.27        | 1.33     |
| 18  | B8    | 232  | GLU  | C-N     | -5.43 | 1.26        | 1.33     |
| 18  | B8    | 1228 | SER  | C-N     | -5.43 | 1.25        | 1.33     |
| 19  | 4     | 122  | GLN  | C-N     | -5.43 | 1.26        | 1.33     |
| 1   | R     | 1252 | VAL  | C-N     | -5.43 | 1.26        | 1.33     |
| 3   | N16   | 210  | THR  | C-N     | -5.43 | 1.26        | 1.33     |
| 10  | C16   | 563  | THR  | C-N     | -5.43 | 1.25        | 1.33     |
| 18  | B8    | 885  | ARG  | C-N     | 5.43  | 1.38        | 1.33     |
| 20  | E     | 494  | ILE  | C-N     | -5.43 | 1.23        | 1.33     |
| 21  | H8    | 163  | PRO  | N-CD    | -5.43 | 1.40        | 1.47     |
| 12  | A48   | 251  | LYS  | C-N     | -5.43 | 1.27        | 1.33     |
| 1   | R16   | 1128 | ALA  | C-N     | -5.42 | 1.26        | 1.33     |
| 18  | B     | 566  | LYS  | C-N     | -5.42 | 1.26        | 1.34     |
| 18  | B     | 817  | CYS  | C-N     | 5.42  | 1.42        | 1.33     |
| 9   | K8    | 639  | THR  | C-N     | -5.42 | 1.26        | 1.33     |
| 11  | A16   | 431  | ARG  | C-N     | -5.42 | 1.26        | 1.33     |
| 18  | B     | 671  | MET  | C-N     | 5.42  | 1.41        | 1.33     |
| 10  | C24   | 448  | LYS  | C-N     | -5.42 | 1.22        | 1.33     |
| 20  | E8    | 180  | THR  | C-N     | -5.42 | 1.26        | 1.33     |
| 21  | H16   | 354  | ASN  | C-N     | -5.42 | 1.27        | 1.33     |
| 24  | D24   | 1440 | PRO  | CA-C    | 5.42  | 1.54        | 1.51     |
| 1   | R16   | 1258 | ALA  | C-N     | 5.42  | 1.41        | 1.33     |
| 1   | R16   | 1440 | PRO  | C-N     | -5.42 | 1.26        | 1.34     |
| 10  | C16   | 1034 | SER  | C-N     | -5.42 | 1.25        | 1.33     |
| 9   | K     | 1089 | LYS  | C-N     | 5.42  | 1.41        | 1.33     |
| 10  | C16   | 1757 | GLN  | C-N     | -5.42 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | M16   | 516  | VAL  | C-N     | -5.41 | 1.26        | 1.33     |
| 6   | O16   | 225  | LYS  | C-N     | -5.41 | 1.25        | 1.33     |
| 19  | 4     | 26   | SER  | C-N     | -5.41 | 1.26        | 1.34     |
| 10  | C32   | 875  | LEU  | C-N     | -5.41 | 1.26        | 1.33     |
| 2   | M16   | 487  | TRP  | C-N     | 5.41  | 1.42        | 1.33     |
| 5   | P     | 622  | ALA  | C-N     | -5.41 | 1.26        | 1.33     |
| 11  | A24   | 781  | LEU  | C-N     | -5.41 | 1.27        | 1.33     |
| 12  | A     | 766  | GLY  | C-N     | -5.41 | 1.25        | 1.33     |
| 11  | A32   | 431  | ARG  | C-N     | -5.41 | 1.26        | 1.33     |
| 1   | R8    | 1128 | ALA  | C-N     | -5.41 | 1.26        | 1.33     |
| 6   | O16   | 222  | PRO  | N-CD    | 5.41  | 1.55        | 1.47     |
| 18  | B     | 1459 | LEU  | C-N     | -5.41 | 1.26        | 1.33     |
| 20  | E8    | 4    | PRO  | C-N     | -5.41 | 1.26        | 1.33     |
| 21  | H8    | 325  | PRO  | C-N     | -5.41 | 1.25        | 1.33     |
| 5   | P     | 123  | GLN  | C-N     | -5.41 | 1.26        | 1.33     |
| 10  | C24   | 817  | HIS  | C-N     | -5.41 | 1.26        | 1.34     |
| 18  | B     | 1667 | ASP  | C-N     | 5.41  | 1.45        | 1.33     |
| 19  | 4     | 88   | ILE  | C-N     | -5.41 | 1.25        | 1.33     |
| 20  | E8    | 120  | ALA  | C-N     | -5.41 | 1.27        | 1.33     |
| 19  | 48    | 88   | ILE  | C-N     | -5.41 | 1.25        | 1.33     |
| 11  | A24   | 810  | PRO  | C-N     | -5.41 | 1.26        | 1.34     |
| 10  | C24   | 1757 | GLN  | C-N     | -5.41 | 1.26        | 1.33     |
| 10  | C     | 929  | LEU  | C-N     | 5.41  | 1.40        | 1.33     |
| 18  | B8    | 12   | TRP  | C-N     | 5.41  | 1.40        | 1.33     |
| 19  | 4     | 249  | PRO  | N-CD    | 5.41  | 1.55        | 1.47     |
| 21  | H     | 325  | PRO  | C-N     | -5.41 | 1.25        | 1.33     |
| 10  | C     | 1424 | GLN  | C-N     | 5.40  | 1.41        | 1.34     |
| 18  | B8    | 699  | MET  | C-N     | -5.40 | 1.27        | 1.33     |
| 19  | 48    | 122  | GLN  | C-N     | -5.40 | 1.26        | 1.33     |
| 2   | M     | 487  | TRP  | C-N     | 5.40  | 1.42        | 1.33     |
| 5   | P8    | 555  | GLU  | C-N     | -5.40 | 1.26        | 1.33     |
| 9   | K8    | 1153 | ALA  | C-N     | -5.40 | 1.25        | 1.33     |
| 11  | A32   | 251  | LYS  | C-N     | -5.40 | 1.27        | 1.33     |
| 22  | I24   | 209  | TRP  | NE1-CE2 | -5.40 | 1.31        | 1.37     |
| 9   | K     | 639  | THR  | C-N     | -5.40 | 1.26        | 1.33     |
| 9   | K8    | 831  | SER  | C-N     | -5.40 | 1.26        | 1.33     |
| 10  | C16   | 1328 | PHE  | C-N     | -5.40 | 1.26        | 1.33     |
| 20  | E8    | 326  | SER  | C-N     | -5.40 | 1.26        | 1.33     |
| 18  | B8    | 363  | PHE  | C-N     | 5.40  | 1.41        | 1.33     |
| 20  | E8    | 215  | GLY  | C-N     | -5.40 | 1.26        | 1.34     |
| 10  | C32   | 1122 | LEU  | C-N     | 5.40  | 1.40        | 1.33     |
| 18  | B8    | 1459 | LEU  | C-N     | -5.40 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | P8    | 604  | TYR  | C-N   | -5.39 | 1.26        | 1.33     |
| 10  | C16   | 875  | LEU  | C-N   | -5.39 | 1.26        | 1.33     |
| 18  | B     | 1802 | ASP  | C-N   | -5.39 | 1.26        | 1.33     |
| 18  | B8    | 671  | MET  | C-N   | 5.39  | 1.41        | 1.33     |
| 20  | E     | 326  | SER  | C-N   | -5.39 | 1.26        | 1.33     |
| 20  | E     | 460  | ALA  | C-N   | -5.39 | 1.26        | 1.33     |
| 10  | C32   | 22   | THR  | C-N   | -5.39 | 1.26        | 1.33     |
| 9   | K     | 838  | GLY  | C-N   | -5.39 | 1.26        | 1.33     |
| 14  | W     | 694  | CYS  | C-N   | -5.39 | 1.26        | 1.33     |
| 18  | B8    | 1034 | ALA  | C-N   | 5.39  | 1.41        | 1.33     |
| 2   | M8    | 536  | ASP  | C-N   | -5.39 | 1.27        | 1.34     |
| 18  | B     | 1228 | SER  | C-N   | -5.39 | 1.25        | 1.33     |
| 18  | B8    | 38   | LYS  | C-N   | -5.39 | 1.26        | 1.33     |
| 5   | P8    | 525  | SER  | C-N   | -5.39 | 1.26        | 1.33     |
| 10  | C16   | 929  | LEU  | C-N   | 5.39  | 1.40        | 1.33     |
| 12  | A     | 251  | LYS  | C-N   | -5.39 | 1.27        | 1.33     |
| 18  | B     | 188  | SER  | C-N   | -5.39 | 1.25        | 1.33     |
| 19  | 48    | 176  | PRO  | N-CD  | -5.39 | 1.40        | 1.47     |
| 12  | A48   | 810  | PRO  | C-N   | -5.39 | 1.26        | 1.34     |
| 2   | M     | 459  | LEU  | C-N   | 5.38  | 1.41        | 1.33     |
| 10  | C8    | 1424 | GLN  | C-N   | 5.38  | 1.41        | 1.34     |
| 20  | E8    | 392  | LEU  | C-N   | -5.38 | 1.25        | 1.33     |
| 5   | P     | 525  | SER  | C-N   | -5.38 | 1.26        | 1.33     |
| 18  | B     | 1724 | MET  | C-N   | -5.38 | 1.26        | 1.33     |
| 18  | B     | 1840 | GLY  | C-N   | -5.38 | 1.27        | 1.33     |
| 9   | K     | 716  | ALA  | C-N   | -5.38 | 1.26        | 1.33     |
| 10  | C8    | 563  | THR  | C-N   | -5.38 | 1.26        | 1.33     |
| 18  | B     | 627  | SER  | C-N   | -5.38 | 1.27        | 1.33     |
| 19  | 4     | 408  | PRO  | N-CD  | 5.38  | 1.55        | 1.47     |
| 10  | C24   | 563  | THR  | C-N   | -5.38 | 1.26        | 1.33     |
| 10  | C     | 1397 | GLU  | C-N   | -5.38 | 1.26        | 1.33     |
| 11  | A24   | 447  | ILE  | C-N   | -5.38 | 1.26        | 1.33     |
| 2   | M     | 536  | ASP  | C-N   | -5.38 | 1.27        | 1.34     |
| 2   | M16   | 695  | HIS  | C-N   | -5.38 | 1.26        | 1.33     |
| 5   | P16   | 583  | GLY  | C-N   | -5.38 | 1.26        | 1.33     |
| 18  | B     | 38   | LYS  | C-N   | -5.38 | 1.26        | 1.33     |
| 20  | E     | 479  | GLU  | C-N   | -5.38 | 1.26        | 1.33     |
| 10  | C32   | 1328 | PHE  | C-N   | -5.38 | 1.26        | 1.33     |
| 9   | K8    | 1089 | LYS  | C-N   | 5.38  | 1.40        | 1.33     |
| 12  | A48   | 766  | GLY  | C-N   | -5.38 | 1.26        | 1.33     |
| 2   | M16   | 536  | ASP  | C-N   | -5.37 | 1.27        | 1.34     |
| 9   | K     | 831  | SER  | C-N   | -5.37 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | K     | 1221 | THR  | C-N     | -5.37 | 1.26        | 1.33     |
| 9   | K8    | 761  | TYR  | C-N     | -5.37 | 1.26        | 1.33     |
| 9   | K8    | 1221 | THR  | C-N     | -5.37 | 1.26        | 1.33     |
| 19  | 4     | 32   | GLU  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C32   | 1034 | SER  | C-N     | -5.37 | 1.25        | 1.33     |
| 2   | M16   | 835  | VAL  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C     | 505  | PHE  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C32   | 817  | HIS  | C-N     | -5.37 | 1.26        | 1.34     |
| 15  | J     | 664  | GLN  | C-N     | -5.37 | 1.27        | 1.33     |
| 10  | C32   | 448  | LYS  | C-N     | -5.37 | 1.22        | 1.33     |
| 1   | R     | 1448 | TRP  | C-N     | -5.37 | 1.26        | 1.33     |
| 13  | V     | 825  | GLN  | C-N     | -5.37 | 1.26        | 1.33     |
| 11  | A16   | 810  | PRO  | C-N     | -5.37 | 1.26        | 1.34     |
| 11  | A32   | 781  | LEU  | C-N     | -5.37 | 1.27        | 1.33     |
| 22  | I     | 209  | TRP  | NE1-CE2 | -5.37 | 1.31        | 1.37     |
| 10  | C32   | 563  | THR  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C16   | 1397 | GLU  | C-N     | -5.37 | 1.26        | 1.33     |
| 20  | E     | 215  | GLY  | C-N     | -5.37 | 1.26        | 1.34     |
| 5   | P16   | 554  | ASP  | C-N     | -5.37 | 1.26        | 1.34     |
| 10  | C24   | 549  | TYR  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C     | 1355 | GLU  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C8    | 419  | SER  | C-N     | -5.37 | 1.26        | 1.33     |
| 10  | C8    | 929  | LEU  | C-N     | 5.37  | 1.40        | 1.33     |
| 18  | B8    | 627  | SER  | C-N     | -5.37 | 1.27        | 1.33     |
| 10  | C32   | 1338 | ASP  | C-N     | 5.37  | 1.38        | 1.33     |
| 6   | O8    | 9    | ASP  | C-N     | -5.36 | 1.26        | 1.33     |
| 9   | K     | 1143 | TRP  | C-N     | -5.36 | 1.26        | 1.34     |
| 9   | K8    | 789  | GLY  | C-N     | -5.36 | 1.26        | 1.34     |
| 9   | K8    | 1204 | THR  | C-N     | 5.36  | 1.41        | 1.34     |
| 11  | A24   | 251  | LYS  | C-N     | -5.36 | 1.27        | 1.33     |
| 11  | A24   | 766  | GLY  | C-N     | -5.36 | 1.26        | 1.33     |
| 10  | C24   | 233  | ASP  | C-N     | -5.36 | 1.27        | 1.33     |
| 20  | E8    | 494  | ILE  | C-N     | -5.36 | 1.23        | 1.33     |
| 10  | C24   | 1397 | GLU  | C-N     | -5.36 | 1.26        | 1.33     |
| 11  | A40   | 447  | ILE  | C-N     | -5.36 | 1.26        | 1.33     |
| 11  | A16   | 671  | GLN  | C-N     | -5.36 | 1.26        | 1.34     |
| 20  | E     | 392  | LEU  | C-N     | -5.36 | 1.25        | 1.33     |
| 5   | P16   | 397  | HIS  | C-N     | -5.36 | 1.26        | 1.33     |
| 9   | K     | 858  | ILE  | C-N     | -5.36 | 1.26        | 1.33     |
| 10  | C24   | 1338 | ASP  | C-N     | 5.36  | 1.38        | 1.33     |
| 10  | C     | 419  | SER  | C-N     | -5.36 | 1.26        | 1.33     |
| 18  | B8    | 1840 | GLY  | C-N     | -5.36 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 13  | V     | 915  | CYS  | C-N   | -5.36 | 1.26        | 1.34     |
| 1   | R     | 1433 | LYS  | C-N   | -5.36 | 1.27        | 1.33     |
| 9   | K8    | 838  | GLY  | C-N   | -5.36 | 1.26        | 1.33     |
| 10  | C24   | 1355 | GLU  | C-N   | -5.36 | 1.26        | 1.33     |
| 10  | C24   | 1556 | ILE  | C-N   | 5.36  | 1.41        | 1.33     |
| 10  | C8    | 1670 | PRO  | C-N   | -5.36 | 1.25        | 1.33     |
| 5   | P16   | 525  | SER  | C-N   | -5.36 | 1.26        | 1.33     |
| 18  | B8    | 1776 | SER  | C-N   | -5.36 | 1.26        | 1.33     |
| 19  | 48    | 428  | CYS  | C-N   | -5.36 | 1.25        | 1.33     |
| 12  | A48   | 671  | GLN  | C-N   | -5.36 | 1.26        | 1.34     |
| 2   | M8    | 695  | HIS  | C-N   | -5.35 | 1.26        | 1.33     |
| 10  | C16   | 609  | SER  | C-N   | -5.35 | 1.27        | 1.33     |
| 18  | B     | 1405 | THR  | C-N   | -5.35 | 1.26        | 1.33     |
| 21  | H16   | 365  | ILE  | C-N   | -5.35 | 1.26        | 1.33     |
| 2   | M     | 788  | PRO  | C-N   | -5.35 | 1.27        | 1.34     |
| 10  | C24   | 505  | PHE  | C-N   | -5.35 | 1.26        | 1.33     |
| 12  | A     | 810  | PRO  | C-N   | -5.35 | 1.26        | 1.34     |
| 18  | B     | 1619 | ILE  | C-N   | 5.35  | 1.41        | 1.33     |
| 18  | B8    | 1440 | ILE  | C-N   | -5.35 | 1.26        | 1.33     |
| 20  | E     | 4    | PRO  | C-N   | -5.35 | 1.26        | 1.33     |
| 20  | E8    | 479  | GLU  | C-N   | -5.35 | 1.26        | 1.33     |
| 21  | H16   | 325  | PRO  | C-N   | -5.35 | 1.25        | 1.33     |
| 12  | A48   | 447  | ILE  | C-N   | -5.35 | 1.26        | 1.33     |
| 13  | V     | 849  | ASP  | C-N   | -5.35 | 1.26        | 1.33     |
| 10  | C24   | 1126 | ASP  | C-N   | -5.35 | 1.26        | 1.33     |
| 11  | A16   | 805  | PHE  | C-N   | -5.35 | 1.26        | 1.33     |
| 9   | K     | 643  | GLY  | C-N   | -5.35 | 1.24        | 1.33     |
| 11  | A24   | 671  | GLN  | C-N   | -5.35 | 1.26        | 1.34     |
| 18  | B     | 832  | LEU  | C-N   | 5.35  | 1.41        | 1.33     |
| 18  | B8    | 188  | SER  | C-N   | -5.35 | 1.25        | 1.33     |
| 19  | 48    | 71   | LYS  | C-N   | 5.35  | 1.40        | 1.33     |
| 10  | C16   | 45   | SER  | C-N   | -5.35 | 1.25        | 1.33     |
| 11  | A16   | 432  | GLN  | C-N   | -5.35 | 1.27        | 1.33     |
| 18  | B     | 129  | ASP  | C-N   | -5.35 | 1.26        | 1.33     |
| 21  | H24   | 325  | PRO  | C-N   | -5.35 | 1.25        | 1.33     |
| 10  | C32   | 461  | THR  | C-N   | -5.35 | 1.26        | 1.33     |
| 2   | M     | 695  | HIS  | C-N   | -5.34 | 1.26        | 1.33     |
| 5   | P     | 554  | ASP  | C-N   | -5.34 | 1.26        | 1.34     |
| 18  | B8    | 553  | LEU  | C-N   | 5.34  | 1.40        | 1.33     |
| 10  | C16   | 1424 | GLN  | C-N   | 5.34  | 1.41        | 1.34     |
| 10  | C16   | 505  | PHE  | C-N   | -5.34 | 1.26        | 1.33     |
| 10  | C     | 875  | LEU  | C-N   | -5.34 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 45   | SER  | C-N   | -5.34 | 1.25        | 1.33     |
| 5   | P16   | 123  | GLN  | C-N   | -5.34 | 1.26        | 1.33     |
| 10  | C16   | 523  | LYS  | C-N   | -5.34 | 1.26        | 1.33     |
| 11  | A16   | 447  | ILE  | C-N   | -5.34 | 1.26        | 1.33     |
| 18  | B     | 200  | PHE  | C-N   | -5.34 | 1.26        | 1.33     |
| 10  | C8    | 1397 | GLU  | C-N   | -5.34 | 1.26        | 1.33     |
| 19  | 4     | 424  | LEU  | C-N   | -5.34 | 1.25        | 1.33     |
| 23  | J24   | 578  | ASN  | C-N   | -5.34 | 1.26        | 1.33     |
| 2   | M     | 853  | GLU  | C-N   | -5.34 | 1.26        | 1.33     |
| 5   | P     | 583  | GLY  | C-N   | -5.34 | 1.26        | 1.33     |
| 10  | C24   | 1424 | GLN  | C-N   | 5.34  | 1.41        | 1.34     |
| 11  | A40   | 251  | LYS  | C-N   | -5.34 | 1.27        | 1.33     |
| 10  | C8    | 194  | TYR  | C-N   | -5.34 | 1.25        | 1.33     |
| 18  | B     | 342  | PRO  | C-N   | 5.34  | 1.40        | 1.33     |
| 12  | A48   | 781  | LEU  | C-N   | -5.34 | 1.27        | 1.33     |
| 9   | K8    | 643  | GLY  | C-N   | -5.33 | 1.24        | 1.33     |
| 10  | C16   | 785  | LEU  | C-N   | -5.33 | 1.26        | 1.33     |
| 11  | A24   | 406  | MET  | C-N   | -5.33 | 1.26        | 1.33     |
| 23  | J32   | 578  | ASN  | C-N   | -5.33 | 1.26        | 1.33     |
| 12  | A     | 781  | LEU  | C-N   | -5.33 | 1.27        | 1.33     |
| 11  | A16   | 781  | LEU  | C-N   | -5.33 | 1.27        | 1.33     |
| 18  | B8    | 1805 | GLU  | C-N   | -5.33 | 1.22        | 1.33     |
| 10  | C32   | 1397 | GLU  | C-N   | -5.33 | 1.26        | 1.33     |
| 9   | K8    | 681  | SER  | C-N   | -5.33 | 1.26        | 1.33     |
| 11  | A40   | 671  | GLN  | C-N   | -5.33 | 1.26        | 1.34     |
| 11  | A32   | 766  | GLY  | C-N   | -5.33 | 1.26        | 1.33     |
| 11  | A24   | 432  | GLN  | C-N   | -5.33 | 1.27        | 1.33     |
| 11  | A16   | 12   | ASP  | C-N   | -5.33 | 1.26        | 1.33     |
| 2   | M     | 207  | SER  | C-N   | 5.33  | 1.41        | 1.33     |
| 10  | C24   | 1328 | PHE  | C-N   | -5.33 | 1.26        | 1.33     |
| 10  | C8    | 1556 | ILE  | C-N   | 5.33  | 1.41        | 1.33     |
| 18  | B8    | 1606 | LYS  | C-N   | 5.33  | 1.41        | 1.33     |
| 2   | M16   | 207  | SER  | C-N   | 5.33  | 1.41        | 1.33     |
| 19  | 4     | 176  | PRO  | N-CD  | -5.33 | 1.40        | 1.47     |
| 2   | M8    | 788  | PRO  | C-N   | -5.33 | 1.27        | 1.34     |
| 6   | O8    | 275  | SER  | C-N   | -5.33 | 1.25        | 1.33     |
| 11  | A24   | 805  | PHE  | C-N   | -5.33 | 1.26        | 1.33     |
| 10  | C24   | 1034 | SER  | C-N   | -5.33 | 1.25        | 1.33     |
| 10  | C     | 22   | THR  | C-N   | -5.33 | 1.26        | 1.33     |
| 10  | C8    | 418  | ASN  | C-N   | 5.33  | 1.41        | 1.34     |
| 19  | 48    | 32   | GLU  | C-N   | -5.32 | 1.27        | 1.33     |
| 19  | 48    | 408  | PRO  | N-CD  | 5.32  | 1.55        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K8    | 1060 | THR  | C-N   | 5.32  | 1.41        | 1.33     |
| 11  | A32   | 671  | GLN  | C-N   | -5.32 | 1.26        | 1.34     |
| 19  | 48    | 424  | LEU  | C-N   | -5.32 | 1.25        | 1.33     |
| 9   | K     | 789  | GLY  | C-N   | -5.32 | 1.26        | 1.34     |
| 10  | C     | 1034 | SER  | C-N   | -5.32 | 1.25        | 1.33     |
| 10  | C8    | 785  | LEU  | C-N   | -5.32 | 1.26        | 1.33     |
| 10  | C8    | 875  | LEU  | C-N   | -5.32 | 1.26        | 1.33     |
| 18  | B8    | 1405 | THR  | C-N   | -5.32 | 1.26        | 1.33     |
| 10  | C16   | 448  | LYS  | C-N   | -5.32 | 1.22        | 1.33     |
| 18  | B8    | 185  | ASP  | C-N   | -5.32 | 1.26        | 1.33     |
| 9   | K     | 673  | SER  | C-N   | -5.31 | 1.26        | 1.33     |
| 10  | C24   | 194  | TYR  | C-N   | -5.31 | 1.26        | 1.33     |
| 1   | R8    | 1448 | TRP  | C-N   | -5.31 | 1.26        | 1.33     |
| 10  | C8    | 538  | PHE  | C-N   | -5.31 | 1.26        | 1.33     |
| 11  | A16   | 251  | LYS  | C-N   | -5.31 | 1.27        | 1.33     |
| 19  | 48    | 249  | PRO  | N-CD  | 5.31  | 1.55        | 1.47     |
| 12  | A48   | 406  | MET  | C-N   | -5.31 | 1.26        | 1.33     |
| 11  | A40   | 12   | ASP  | C-N   | -5.31 | 1.26        | 1.33     |
| 10  | C32   | 785  | LEU  | C-N   | -5.31 | 1.26        | 1.33     |
| 1   | R16   | 1165 | MET  | C-N   | 5.31  | 1.41        | 1.33     |
| 2   | M16   | 788  | PRO  | C-N   | -5.31 | 1.27        | 1.34     |
| 7   | Q16   | 239  | ARG  | C-N   | -5.31 | 1.25        | 1.33     |
| 12  | A48   | 507  | VAL  | C-N   | -5.31 | 1.26        | 1.33     |
| 6   | O     | 9    | ASP  | C-N   | -5.31 | 1.26        | 1.33     |
| 10  | C16   | 419  | SER  | C-N   | -5.31 | 1.26        | 1.33     |
| 12  | A     | 671  | GLN  | C-N   | -5.31 | 1.26        | 1.34     |
| 10  | C     | 1650 | ASN  | C-N   | 5.31  | 1.41        | 1.33     |
| 11  | A16   | 406  | MET  | C-N   | -5.31 | 1.26        | 1.33     |
| 18  | B8    | 200  | PHE  | C-N   | -5.31 | 1.26        | 1.33     |
| 19  | 4     | 71   | LYS  | C-N   | 5.31  | 1.39        | 1.33     |
| 2   | M8    | 207  | SER  | C-N   | 5.31  | 1.41        | 1.33     |
| 5   | P     | 341  | MET  | C-N   | 5.31  | 1.41        | 1.34     |
| 5   | P8    | 123  | GLN  | C-N   | -5.30 | 1.26        | 1.33     |
| 9   | K     | 681  | SER  | C-N   | -5.30 | 1.26        | 1.33     |
| 9   | K8    | 854  | SER  | C-N   | 5.30  | 1.41        | 1.33     |
| 10  | C24   | 698  | PHE  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C     | 1761 | HIS  | C-N   | -5.30 | 1.27        | 1.33     |
| 18  | B     | 185  | ASP  | C-N   | -5.30 | 1.26        | 1.33     |
| 18  | B     | 1440 | ILE  | C-N   | -5.30 | 1.26        | 1.33     |
| 19  | 4     | 17   | ARG  | C-N   | -5.30 | 1.26        | 1.33     |
| 19  | 4     | 428  | CYS  | C-N   | -5.30 | 1.25        | 1.33     |
| 10  | C24   | 22   | THR  | C-N   | -5.30 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23  | J32   | 712  | GLU  | C-N   | -5.30 | 1.26        | 1.33     |
| 11  | A40   | 507  | VAL  | C-N   | -5.30 | 1.26        | 1.33     |
| 18  | B8    | 1519 | ASP  | C-N   | -5.30 | 1.26        | 1.33     |
| 19  | 48    | 344  | PRO  | C-N   | -5.30 | 1.26        | 1.33     |
| 20  | E8    | 6    | VAL  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C32   | 1670 | PRO  | C-N   | -5.30 | 1.25        | 1.33     |
| 2   | M8    | 853  | GLU  | C-N   | -5.30 | 1.26        | 1.33     |
| 9   | K     | 761  | TYR  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C     | 1670 | PRO  | C-N   | -5.30 | 1.25        | 1.33     |
| 10  | C     | 1810 | LEU  | C-N   | -5.30 | 1.26        | 1.33     |
| 18  | B8    | 832  | LEU  | C-N   | 5.30  | 1.40        | 1.33     |
| 10  | C16   | 1810 | LEU  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C16   | 538  | PHE  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C     | 1556 | ILE  | C-N   | 5.30  | 1.40        | 1.33     |
| 18  | B     | 1805 | GLU  | C-N   | -5.30 | 1.22        | 1.33     |
| 20  | E     | 6    | VAL  | C-N   | -5.30 | 1.26        | 1.33     |
| 10  | C24   | 1810 | LEU  | C-N   | -5.29 | 1.26        | 1.33     |
| 18  | B     | 1014 | ASP  | C-N   | 5.29  | 1.40        | 1.33     |
| 20  | E8    | 311  | LYS  | C-N   | -5.29 | 1.27        | 1.33     |
| 1   | R8    | 1165 | MET  | C-N   | 5.29  | 1.41        | 1.33     |
| 9   | K     | 1060 | THR  | C-N   | 5.29  | 1.41        | 1.33     |
| 3   | N     | 256  | LYS  | C-N   | -5.29 | 1.25        | 1.33     |
| 10  | C24   | 461  | THR  | C-N   | -5.29 | 1.26        | 1.33     |
| 13  | V     | 731  | PRO  | C-N   | -5.29 | 1.26        | 1.34     |
| 11  | A16   | 791  | PRO  | C-N   | 5.29  | 1.40        | 1.33     |
| 18  | B8    | 129  | ASP  | C-N   | -5.29 | 1.26        | 1.33     |
| 20  | E     | 508  | LEU  | C-N   | -5.29 | 1.27        | 1.33     |
| 5   | P8    | 554  | ASP  | C-N   | -5.29 | 1.26        | 1.34     |
| 10  | C16   | 22   | THR  | C-N   | -5.29 | 1.26        | 1.33     |
| 11  | A32   | 507  | VAL  | C-N   | -5.29 | 1.27        | 1.33     |
| 11  | A32   | 805  | PHE  | C-N   | -5.29 | 1.27        | 1.33     |
| 10  | C32   | 1650 | ASN  | C-N   | 5.29  | 1.41        | 1.33     |
| 5   | P16   | 341  | MET  | C-N   | 5.29  | 1.41        | 1.34     |
| 10  | C8    | 1034 | SER  | C-N   | -5.29 | 1.25        | 1.33     |
| 23  | J8    | 578  | ASN  | C-N   | -5.29 | 1.27        | 1.33     |
| 10  | C32   | 1355 | GLU  | C-N   | -5.29 | 1.26        | 1.33     |
| 10  | C24   | 45   | SER  | C-N   | -5.29 | 1.25        | 1.33     |
| 10  | C8    | 427  | ASP  | C-N   | -5.29 | 1.25        | 1.33     |
| 23  | J16   | 578  | ASN  | C-N   | -5.29 | 1.27        | 1.33     |
| 10  | C32   | 929  | LEU  | C-N   | 5.29  | 1.40        | 1.33     |
| 10  | C8    | 461  | THR  | C-N   | -5.29 | 1.26        | 1.33     |
| 18  | B     | 553  | LEU  | C-N   | 5.29  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 1069 | VAL  | C-N   | 5.29  | 1.40        | 1.33     |
| 20  | E     | 131  | PRO  | C-N   | 5.29  | 1.40        | 1.33     |
| 2   | M     | 811  | SER  | C-N   | 5.28  | 1.41        | 1.33     |
| 10  | C24   | 427  | ASP  | C-N   | -5.28 | 1.25        | 1.33     |
| 10  | C     | 418  | ASN  | C-N   | 5.28  | 1.41        | 1.34     |
| 18  | B8    | 33   | PRO  | N-CD  | -5.28 | 1.40        | 1.47     |
| 20  | E8    | 411  | GLU  | C-N   | -5.28 | 1.27        | 1.33     |
| 23  | J32   | 672  | VAL  | C-N   | -5.28 | 1.27        | 1.33     |
| 10  | C32   | 418  | ASN  | C-N   | 5.28  | 1.41        | 1.34     |
| 1   | R     | 1165 | MET  | C-N   | 5.28  | 1.41        | 1.33     |
| 3   | N8    | 256  | LYS  | C-N   | -5.28 | 1.25        | 1.33     |
| 18  | B     | 1390 | LEU  | C-N   | 5.28  | 1.41        | 1.33     |
| 3   | N16   | 256  | LYS  | C-N   | -5.28 | 1.25        | 1.33     |
| 5   | P16   | 159  | ILE  | C-N   | -5.28 | 1.26        | 1.33     |
| 10  | C16   | 1355 | GLU  | C-N   | -5.28 | 1.26        | 1.33     |
| 15  | J     | 708  | GLU  | C-N   | -5.28 | 1.26        | 1.33     |
| 18  | B     | 65   | LEU  | C-N   | 5.28  | 1.41        | 1.33     |
| 18  | B     | 885  | ARG  | C-N   | 5.28  | 1.38        | 1.33     |
| 18  | B     | 961  | PRO  | N-CD  | -5.28 | 1.40        | 1.47     |
| 19  | 4     | 344  | PRO  | C-N   | -5.28 | 1.26        | 1.33     |
| 10  | C32   | 1556 | ILE  | C-N   | 5.28  | 1.40        | 1.33     |
| 10  | C16   | 1670 | PRO  | C-N   | -5.28 | 1.25        | 1.33     |
| 19  | 48    | 296  | GLY  | C-N   | -5.28 | 1.25        | 1.33     |
| 10  | C32   | 1756 | LEU  | C-N   | -5.28 | 1.26        | 1.33     |
| 2   | M     | 673  | ASN  | C-N   | 5.28  | 1.41        | 1.34     |
| 18  | B8    | 1014 | ASP  | C-N   | 5.28  | 1.40        | 1.33     |
| 20  | E8    | 508  | LEU  | C-N   | -5.28 | 1.27        | 1.33     |
| 1   | R     | 1344 | ILE  | C-N   | 5.27  | 1.41        | 1.33     |
| 9   | K     | 670  | LEU  | C-N   | -5.27 | 1.26        | 1.33     |
| 10  | C16   | 194  | TYR  | C-N   | -5.27 | 1.26        | 1.33     |
| 10  | C16   | 549  | TYR  | C-N   | -5.27 | 1.26        | 1.33     |
| 10  | C24   | 419  | SER  | C-N   | -5.27 | 1.26        | 1.33     |
| 13  | V     | 822  | GLN  | C-N   | -5.27 | 1.26        | 1.34     |
| 18  | B     | 699  | MET  | C-N   | -5.27 | 1.27        | 1.33     |
| 18  | B8    | 1164 | GLU  | C-N   | -5.27 | 1.26        | 1.34     |
| 2   | M16   | 811  | SER  | C-N   | 5.27  | 1.41        | 1.33     |
| 2   | M16   | 853  | GLU  | C-N   | -5.27 | 1.26        | 1.33     |
| 10  | C16   | 1761 | HIS  | C-N   | -5.27 | 1.27        | 1.33     |
| 21  | H     | 365  | ILE  | C-N   | -5.27 | 1.26        | 1.33     |
| 22  | I     | 339  | ASP  | C-N   | -5.27 | 1.26        | 1.33     |
| 5   | P8    | 606  | ASP  | C-N   | -5.27 | 1.26        | 1.33     |
| 11  | A32   | 23   | GLN  | C-N   | 5.27  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 24  | D32   | 385  | PRO  | CA-C  | 5.27  | 1.54        | 1.51     |
| 1   | R16   | 1433 | LYS  | C-N   | -5.27 | 1.27        | 1.33     |
| 5   | P8    | 615  | HIS  | C-N   | -5.27 | 1.25        | 1.33     |
| 6   | O8    | 190  | ALA  | C-N   | 5.27  | 1.41        | 1.33     |
| 9   | K8    | 673  | SER  | C-N   | -5.27 | 1.26        | 1.33     |
| 11  | A24   | 791  | PRO  | C-N   | 5.27  | 1.40        | 1.33     |
| 11  | A40   | 406  | MET  | C-N   | -5.27 | 1.26        | 1.33     |
| 10  | C     | 538  | PHE  | C-N   | -5.27 | 1.26        | 1.33     |
| 3   | N16   | 164  | PRO  | C-N   | -5.27 | 1.24        | 1.33     |
| 3   | N16   | 299  | ALA  | C-N   | 5.27  | 1.41        | 1.33     |
| 5   | P     | 615  | HIS  | C-N   | -5.27 | 1.25        | 1.33     |
| 9   | K     | 733  | LEU  | C-N   | -5.27 | 1.27        | 1.33     |
| 9   | K8    | 672  | LEU  | C-N   | -5.27 | 1.25        | 1.33     |
| 10  | C16   | 1756 | LEU  | C-N   | -5.27 | 1.26        | 1.33     |
| 18  | B     | 1783 | VAL  | C-N   | -5.27 | 1.25        | 1.33     |
| 3   | N     | 164  | PRO  | C-N   | -5.27 | 1.24        | 1.33     |
| 10  | C24   | 1138 | GLU  | C-N   | 5.27  | 1.41        | 1.33     |
| 1   | R8    | 1433 | LYS  | C-N   | -5.26 | 1.27        | 1.33     |
| 12  | A     | 406  | MET  | C-N   | -5.26 | 1.26        | 1.33     |
| 10  | C8    | 1126 | ASP  | C-N   | -5.26 | 1.26        | 1.33     |
| 10  | C8    | 1650 | ASN  | C-N   | 5.26  | 1.41        | 1.33     |
| 11  | A32   | 360  | GLU  | C-N   | -5.26 | 1.27        | 1.33     |
| 18  | B8    | 1528 | PRO  | C-N   | 5.26  | 1.41        | 1.33     |
| 19  | 48    | 17   | ARG  | C-N   | -5.26 | 1.26        | 1.33     |
| 10  | C32   | 288  | GLN  | C-N   | 5.26  | 1.41        | 1.33     |
| 2   | M8    | 214  | SER  | C-N   | -5.26 | 1.25        | 1.33     |
| 5   | P8    | 341  | MET  | C-N   | 5.26  | 1.41        | 1.34     |
| 9   | K8    | 733  | LEU  | C-N   | -5.26 | 1.27        | 1.33     |
| 19  | 4     | 286  | TRP  | C-N   | -5.26 | 1.25        | 1.33     |
| 19  | 4     | 296  | GLY  | C-N   | -5.26 | 1.25        | 1.33     |
| 10  | C32   | 538  | PHE  | C-N   | -5.26 | 1.26        | 1.33     |
| 12  | A48   | 791  | PRO  | C-N   | 5.26  | 1.40        | 1.33     |
| 9   | K8    | 585  | GLU  | C-N   | -5.26 | 1.27        | 1.33     |
| 15  | J     | 686  | MET  | C-N   | -5.26 | 1.24        | 1.33     |
| 10  | C8    | 1355 | GLU  | C-N   | -5.26 | 1.26        | 1.33     |
| 18  | B     | 1069 | VAL  | C-N   | 5.26  | 1.40        | 1.33     |
| 20  | E     | 411  | GLU  | C-N   | -5.26 | 1.27        | 1.33     |
| 10  | C32   | 419  | SER  | C-N   | -5.26 | 1.26        | 1.33     |
| 10  | C24   | 929  | LEU  | C-N   | 5.26  | 1.40        | 1.33     |
| 10  | C8    | 1743 | GLN  | C-N   | -5.26 | 1.27        | 1.33     |
| 18  | B8    | 1590 | LEU  | C-N   | 5.26  | 1.41        | 1.33     |
| 5   | P     | 128  | GLU  | C-N   | -5.26 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C8    | 45   | SER  | C-N   | -5.26 | 1.25        | 1.33     |
| 18  | B     | 1766 | SER  | C-N   | -5.26 | 1.25        | 1.33     |
| 9   | K8    | 670  | LEU  | C-N   | -5.26 | 1.26        | 1.33     |
| 10  | C8    | 288  | GLN  | C-N   | 5.26  | 1.41        | 1.33     |
| 10  | C16   | 817  | HIS  | C-N   | -5.25 | 1.26        | 1.34     |
| 10  | C8    | 22   | THR  | C-N   | -5.25 | 1.26        | 1.33     |
| 20  | E     | 311  | LYS  | C-N   | -5.25 | 1.27        | 1.33     |
| 11  | A24   | 12   | ASP  | C-N   | -5.25 | 1.26        | 1.33     |
| 11  | A40   | 805  | PHE  | C-N   | -5.25 | 1.27        | 1.33     |
| 11  | A16   | 23   | GLN  | C-N   | 5.25  | 1.41        | 1.33     |
| 18  | B     | 1519 | ASP  | C-N   | -5.25 | 1.26        | 1.33     |
| 22  | I16   | 196  | VAL  | C-N   | -5.25 | 1.26        | 1.33     |
| 7   | Q16   | 301  | ARG  | C-N   | 5.25  | 1.40        | 1.33     |
| 10  | C24   | 1761 | HIS  | C-N   | -5.25 | 1.27        | 1.33     |
| 10  | C     | 427  | ASP  | C-N   | -5.25 | 1.25        | 1.33     |
| 18  | B     | 204  | ALA  | C-N   | -5.25 | 1.27        | 1.33     |
| 18  | B8    | 204  | ALA  | C-N   | -5.25 | 1.27        | 1.33     |
| 22  | I8    | 327  | GLN  | C-N   | -5.25 | 1.26        | 1.33     |
| 2   | M     | 741  | SER  | C-N   | -5.25 | 1.27        | 1.33     |
| 6   | O16   | 9    | ASP  | C-N   | -5.25 | 1.26        | 1.33     |
| 11  | A16   | 766  | GLY  | C-N   | -5.25 | 1.26        | 1.33     |
| 18  | B     | 1606 | LYS  | C-N   | 5.25  | 1.41        | 1.33     |
| 22  | I24   | 196  | VAL  | C-N   | -5.25 | 1.26        | 1.33     |
| 2   | M8    | 811  | SER  | C-N   | 5.25  | 1.41        | 1.33     |
| 2   | M16   | 214  | SER  | C-N   | -5.25 | 1.25        | 1.33     |
| 5   | P     | 217  | PHE  | C-N   | -5.25 | 1.27        | 1.33     |
| 15  | J     | 590  | ALA  | C-N   | -5.25 | 1.26        | 1.33     |
| 10  | C     | 575  | PHE  | C-N   | -5.25 | 1.25        | 1.33     |
| 21  | H8    | 365  | ILE  | C-N   | -5.25 | 1.26        | 1.33     |
| 1   | R16   | 1448 | TRP  | C-N   | -5.25 | 1.26        | 1.33     |
| 11  | A24   | 507  | VAL  | C-N   | -5.25 | 1.27        | 1.33     |
| 11  | A40   | 766  | GLY  | C-N   | -5.25 | 1.26        | 1.33     |
| 18  | B     | 1109 | SER  | C-N   | -5.25 | 1.25        | 1.33     |
| 10  | C32   | 788  | LEU  | C-N   | -5.25 | 1.27        | 1.33     |
| 10  | C32   | 1761 | HIS  | C-N   | -5.25 | 1.27        | 1.33     |
| 3   | N8    | 164  | PRO  | C-N   | -5.25 | 1.25        | 1.33     |
| 10  | C16   | 461  | THR  | C-N   | -5.25 | 1.26        | 1.33     |
| 10  | C     | 461  | THR  | C-N   | -5.25 | 1.26        | 1.33     |
| 23  | J16   | 672  | VAL  | C-N   | -5.25 | 1.27        | 1.33     |
| 10  | C     | 1298 | SER  | C-N   | -5.24 | 1.27        | 1.33     |
| 10  | C     | 1496 | PHE  | C-N   | 5.24  | 1.40        | 1.33     |
| 10  | C8    | 1187 | GLY  | C-N   | -5.24 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 12  | A     | 360  | GLU  | C-N   | -5.24 | 1.27        | 1.33     |
| 19  | 48    | 286  | TRP  | C-N   | -5.24 | 1.25        | 1.33     |
| 2   | M16   | 673  | ASN  | C-N   | 5.24  | 1.41        | 1.34     |
| 7   | Q8    | 301  | ARG  | C-N   | 5.24  | 1.40        | 1.33     |
| 10  | C24   | 248  | LEU  | C-N   | 5.24  | 1.40        | 1.33     |
| 12  | A     | 805  | PHE  | C-N   | -5.24 | 1.27        | 1.33     |
| 11  | A32   | 791  | PRO  | C-N   | 5.24  | 1.40        | 1.33     |
| 18  | B8    | 1791 | VAL  | C-N   | -5.24 | 1.26        | 1.33     |
| 22  | I16   | 339  | ASP  | C-N   | -5.24 | 1.26        | 1.33     |
| 10  | C32   | 428  | GLY  | C-N   | 5.24  | 1.40        | 1.33     |
| 2   | M16   | 340  | GLU  | C-N   | -5.24 | 1.26        | 1.33     |
| 9   | K     | 885  | ALA  | C-N   | -5.24 | 1.26        | 1.34     |
| 10  | C24   | 770  | SER  | C-N   | 5.24  | 1.41        | 1.33     |
| 10  | C     | 785  | LEU  | C-N   | -5.24 | 1.27        | 1.33     |
| 10  | C8    | 1761 | HIS  | C-N   | -5.24 | 1.27        | 1.33     |
| 10  | C8    | 1810 | LEU  | C-N   | -5.24 | 1.26        | 1.33     |
| 18  | B     | 1791 | VAL  | C-N   | -5.24 | 1.26        | 1.33     |
| 22  | I8    | 339  | ASP  | C-N   | -5.24 | 1.26        | 1.33     |
| 10  | C16   | 418  | ASN  | C-N   | 5.24  | 1.41        | 1.34     |
| 10  | C16   | 1721 | GLN  | C-N   | 5.24  | 1.40        | 1.33     |
| 5   | P8    | 646  | PRO  | C-N   | -5.24 | 1.27        | 1.33     |
| 5   | P16   | 217  | PHE  | C-N   | -5.24 | 1.27        | 1.33     |
| 9   | K8    | 716  | ALA  | C-N   | -5.24 | 1.26        | 1.33     |
| 10  | C     | 591  | ALA  | C-N   | 5.24  | 1.40        | 1.33     |
| 18  | B     | 1776 | SER  | C-N   | -5.24 | 1.26        | 1.33     |
| 19  | 4     | 241  | ASP  | C-N   | -5.24 | 1.27        | 1.33     |
| 10  | C16   | 452  | LEU  | C-N   | 5.23  | 1.40        | 1.33     |
| 10  | C16   | 1650 | ASN  | C-N   | 5.23  | 1.41        | 1.33     |
| 10  | C24   | 538  | PHE  | C-N   | -5.23 | 1.26        | 1.33     |
| 12  | A     | 507  | VAL  | C-N   | -5.23 | 1.27        | 1.33     |
| 11  | A32   | 12   | ASP  | C-N   | -5.23 | 1.26        | 1.33     |
| 2   | M     | 266  | PHE  | C-N   | -5.23 | 1.25        | 1.33     |
| 6   | O16   | 275  | SER  | C-N   | -5.23 | 1.25        | 1.33     |
| 10  | C16   | 1556 | ILE  | C-N   | 5.23  | 1.40        | 1.33     |
| 18  | B8    | 961  | PRO  | N-CD  | -5.23 | 1.40        | 1.47     |
| 23  | J24   | 672  | VAL  | C-N   | -5.23 | 1.27        | 1.33     |
| 2   | M     | 835  | VAL  | C-N   | -5.23 | 1.27        | 1.33     |
| 10  | C16   | 427  | ASP  | C-N   | -5.23 | 1.25        | 1.33     |
| 18  | B8    | 1214 | ALA  | C-N   | -5.23 | 1.26        | 1.33     |
| 19  | 48    | 425  | LEU  | C-N   | -5.23 | 1.25        | 1.33     |
| 22  | I     | 327  | GLN  | C-N   | -5.23 | 1.26        | 1.33     |
| 23  | J8    | 712  | GLU  | C-N   | -5.23 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 523  | LYS  | C-N   | -5.23 | 1.26        | 1.33     |
| 2   | M     | 214  | SER  | C-N   | -5.23 | 1.25        | 1.33     |
| 9   | K     | 854  | SER  | C-N   | 5.23  | 1.41        | 1.33     |
| 10  | C24   | 1650 | ASN  | C-N   | 5.23  | 1.41        | 1.33     |
| 18  | B     | 33   | PRO  | N-CD  | -5.23 | 1.40        | 1.47     |
| 18  | B     | 882  | SER  | C-N   | 5.23  | 1.40        | 1.33     |
| 1   | R8    | 1344 | ILE  | C-N   | 5.23  | 1.41        | 1.33     |
| 7   | Q     | 301  | ARG  | C-N   | 5.23  | 1.40        | 1.33     |
| 13  | V     | 879  | ARG  | C-N   | 5.23  | 1.41        | 1.33     |
| 10  | C16   | 288  | GLN  | C-N   | 5.23  | 1.41        | 1.33     |
| 10  | C     | 1657 | SER  | C-N   | -5.23 | 1.26        | 1.33     |
| 10  | C8    | 1602 | GLY  | C-N   | 5.23  | 1.40        | 1.33     |
| 10  | C32   | 427  | ASP  | C-N   | -5.23 | 1.25        | 1.33     |
| 10  | C16   | 1298 | SER  | C-N   | -5.22 | 1.27        | 1.33     |
| 10  | C     | 45   | SER  | C-N   | -5.22 | 1.25        | 1.33     |
| 22  | I     | 196  | VAL  | C-N   | -5.22 | 1.26        | 1.33     |
| 23  | J24   | 712  | GLU  | C-N   | -5.22 | 1.27        | 1.33     |
| 12  | A48   | 782  | PRO  | C-N   | -5.22 | 1.26        | 1.33     |
| 2   | M8    | 766  | ASN  | C-N   | -5.22 | 1.26        | 1.33     |
| 2   | M16   | 766  | ASN  | C-N   | -5.22 | 1.26        | 1.33     |
| 10  | C16   | 1496 | PHE  | C-N   | 5.22  | 1.40        | 1.33     |
| 10  | C24   | 400  | PRO  | C-N   | 5.22  | 1.40        | 1.33     |
| 18  | B8    | 65   | LEU  | C-N   | 5.22  | 1.41        | 1.33     |
| 20  | E8    | 260  | ASN  | C-N   | -5.22 | 1.27        | 1.34     |
| 5   | P16   | 646  | PRO  | C-N   | -5.22 | 1.27        | 1.33     |
| 11  | A40   | 782  | PRO  | C-N   | -5.22 | 1.26        | 1.33     |
| 10  | C8    | 1695 | LEU  | C-N   | -5.22 | 1.27        | 1.33     |
| 10  | C32   | 93   | ASP  | C-N   | -5.22 | 1.26        | 1.33     |
| 2   | M8    | 266  | PHE  | C-N   | -5.22 | 1.25        | 1.33     |
| 10  | C8    | 746  | GLY  | C-N   | -5.22 | 1.26        | 1.33     |
| 18  | B     | 160  | GLU  | C-N   | -5.22 | 1.26        | 1.33     |
| 18  | B     | 1214 | ALA  | C-N   | -5.22 | 1.26        | 1.33     |
| 10  | C32   | 452  | LEU  | C-N   | 5.22  | 1.40        | 1.33     |
| 10  | C32   | 1721 | GLN  | C-N   | 5.22  | 1.40        | 1.33     |
| 2   | M8    | 825  | THR  | C-N   | -5.22 | 1.26        | 1.34     |
| 5   | P16   | 61   | ASP  | C-N   | 5.22  | 1.40        | 1.33     |
| 9   | K     | 672  | LEU  | C-N   | -5.22 | 1.25        | 1.33     |
| 23  | J32   | 606  | ILE  | C-N   | -5.22 | 1.27        | 1.33     |
| 2   | M     | 766  | ASN  | C-N   | -5.22 | 1.26        | 1.33     |
| 3   | N8    | 299  | ALA  | C-N   | 5.22  | 1.41        | 1.33     |
| 18  | B     | 727  | GLY  | C-N   | 5.22  | 1.40        | 1.33     |
| 18  | B8    | 342  | PRO  | C-N   | 5.22  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B8    | 1109 | SER  | C-N   | -5.22 | 1.25        | 1.33     |
| 18  | B8    | 1766 | SER  | C-N   | -5.22 | 1.26        | 1.33     |
| 22  | I24   | 339  | ASP  | C-N   | -5.22 | 1.26        | 1.33     |
| 10  | C32   | 1496 | PHE  | C-N   | 5.22  | 1.40        | 1.33     |
| 10  | C32   | 1810 | LEU  | C-N   | -5.22 | 1.26        | 1.33     |
| 1   | R16   | 1344 | ILE  | C-N   | 5.21  | 1.41        | 1.33     |
| 6   | O     | 275  | SER  | C-N   | -5.21 | 1.25        | 1.33     |
| 11  | A40   | 23   | GLN  | C-N   | 5.21  | 1.41        | 1.33     |
| 15  | J     | 661  | MET  | C-N   | -5.21 | 1.27        | 1.33     |
| 10  | C8    | 575  | PHE  | C-N   | -5.21 | 1.25        | 1.33     |
| 10  | C8    | 817  | HIS  | C-N   | -5.21 | 1.26        | 1.34     |
| 19  | 48    | 241  | ASP  | C-N   | -5.21 | 1.27        | 1.33     |
| 10  | C32   | 1138 | GLU  | C-N   | 5.21  | 1.41        | 1.33     |
| 10  | C32   | 1674 | LEU  | C-N   | -5.21 | 1.27        | 1.33     |
| 10  | C     | 1126 | ASP  | C-N   | -5.21 | 1.26        | 1.33     |
| 11  | A24   | 23   | GLN  | C-N   | 5.21  | 1.41        | 1.33     |
| 10  | C     | 194  | TYR  | C-N   | -5.21 | 1.26        | 1.33     |
| 10  | C     | 817  | HIS  | C-N   | -5.21 | 1.26        | 1.34     |
| 11  | A16   | 507  | VAL  | C-N   | -5.21 | 1.27        | 1.33     |
| 21  | H24   | 365  | ILE  | C-N   | -5.21 | 1.26        | 1.33     |
| 2   | M8    | 835  | VAL  | C-N   | -5.21 | 1.27        | 1.33     |
| 10  | C24   | 288  | GLN  | C-N   | 5.21  | 1.41        | 1.33     |
| 10  | C24   | 523  | LYS  | C-N   | -5.21 | 1.26        | 1.33     |
| 10  | C8    | 1483 | GLY  | C-N   | 5.21  | 1.40        | 1.33     |
| 10  | C32   | 194  | TYR  | C-N   | -5.21 | 1.26        | 1.33     |
| 2   | M16   | 526  | ASP  | C-N   | -5.21 | 1.25        | 1.33     |
| 6   | O16   | 207  | ASP  | C-N   | -5.21 | 1.26        | 1.34     |
| 10  | C24   | 1496 | PHE  | C-N   | 5.21  | 1.40        | 1.33     |
| 10  | C     | 1756 | LEU  | C-N   | -5.21 | 1.26        | 1.33     |
| 10  | C8    | 1496 | PHE  | C-N   | 5.21  | 1.40        | 1.33     |
| 18  | B     | 464  | ALA  | C-N   | 5.21  | 1.41        | 1.33     |
| 18  | B8    | 390  | HIS  | C-N   | -5.21 | 1.26        | 1.33     |
| 18  | B8    | 882  | SER  | C-N   | 5.21  | 1.40        | 1.33     |
| 12  | A48   | 805  | PHE  | C-N   | -5.21 | 1.27        | 1.33     |
| 10  | C24   | 1670 | PRO  | C-N   | -5.21 | 1.25        | 1.33     |
| 10  | C8    | 591  | ALA  | C-N   | 5.21  | 1.40        | 1.33     |
| 23  | J8    | 606  | ILE  | C-N   | -5.21 | 1.27        | 1.33     |
| 6   | O     | 190  | ALA  | C-N   | 5.20  | 1.41        | 1.33     |
| 5   | P8    | 217  | PHE  | C-N   | -5.20 | 1.27        | 1.33     |
| 10  | C16   | 93   | ASP  | C-N   | -5.20 | 1.26        | 1.33     |
| 10  | C16   | 1126 | ASP  | C-N   | -5.20 | 1.26        | 1.33     |
| 10  | C     | 288  | GLN  | C-N   | 5.20  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 759  | MET  | C-N   | -5.20 | 1.27        | 1.33     |
| 18  | B8    | 1783 | VAL  | C-N   | -5.20 | 1.25        | 1.33     |
| 20  | E8    | 131  | PRO  | C-N   | 5.20  | 1.40        | 1.33     |
| 10  | C32   | 1126 | ASP  | C-N   | -5.20 | 1.26        | 1.33     |
| 22  | I16   | 327  | GLN  | C-N   | -5.20 | 1.26        | 1.33     |
| 2   | M     | 526  | ASP  | C-N   | -5.20 | 1.25        | 1.33     |
| 11  | A40   | 360  | GLU  | C-N   | -5.20 | 1.27        | 1.33     |
| 14  | W     | 759  | GLN  | C-N   | 5.20  | 1.41        | 1.33     |
| 10  | C8    | 788  | LEU  | C-N   | -5.20 | 1.27        | 1.33     |
| 18  | B     | 85   | ASP  | C-N   | -5.20 | 1.26        | 1.33     |
| 22  | I8    | 196  | VAL  | C-N   | -5.20 | 1.26        | 1.33     |
| 23  | J16   | 712  | GLU  | C-N   | -5.20 | 1.27        | 1.33     |
| 6   | O     | 207  | ASP  | C-N   | -5.20 | 1.26        | 1.34     |
| 10  | C     | 122  | LEU  | C-N   | 5.20  | 1.40        | 1.33     |
| 11  | A16   | 360  | GLU  | C-N   | -5.20 | 1.27        | 1.33     |
| 18  | B8    | 759  | MET  | C-N   | -5.20 | 1.27        | 1.33     |
| 23  | J8    | 672  | VAL  | C-N   | -5.20 | 1.27        | 1.33     |
| 10  | C24   | 1298 | SER  | C-N   | -5.20 | 1.27        | 1.33     |
| 22  | I24   | 327  | GLN  | C-N   | -5.20 | 1.26        | 1.33     |
| 1   | R     | 1325 | GLN  | C-N   | -5.20 | 1.26        | 1.33     |
| 2   | M8    | 526  | ASP  | C-N   | -5.20 | 1.25        | 1.33     |
| 2   | M8    | 741  | SER  | C-N   | -5.20 | 1.27        | 1.33     |
| 10  | C24   | 1743 | GLN  | C-N   | -5.20 | 1.27        | 1.33     |
| 11  | A32   | 447  | ILE  | C-N   | -5.20 | 1.26        | 1.33     |
| 18  | B     | 390  | HIS  | C-N   | -5.20 | 1.26        | 1.33     |
| 10  | C32   | 549  | TYR  | C-N   | -5.20 | 1.26        | 1.33     |
| 2   | M8    | 801  | GLU  | C-N   | -5.19 | 1.27        | 1.33     |
| 5   | P16   | 606  | ASP  | C-N   | -5.19 | 1.26        | 1.33     |
| 2   | M16   | 801  | GLU  | C-N   | -5.19 | 1.27        | 1.33     |
| 10  | C16   | 746  | GLY  | C-N   | -5.19 | 1.26        | 1.33     |
| 23  | J8    | 584  | ARG  | C-N   | -5.19 | 1.27        | 1.33     |
| 10  | C32   | 248  | LEU  | C-N   | 5.19  | 1.40        | 1.33     |
| 1   | R16   | 1325 | GLN  | C-N   | -5.19 | 1.26        | 1.33     |
| 5   | P     | 125  | ALA  | C-N   | -5.19 | 1.27        | 1.33     |
| 5   | P     | 444  | LEU  | C-N   | -5.19 | 1.27        | 1.33     |
| 6   | O16   | 190  | ALA  | C-N   | 5.19  | 1.41        | 1.33     |
| 10  | C8    | 1685 | SER  | C-N   | -5.19 | 1.27        | 1.33     |
| 18  | B8    | 160  | GLU  | C-N   | -5.19 | 1.26        | 1.33     |
| 18  | B8    | 1910 | GLU  | C-N   | -5.19 | 1.27        | 1.33     |
| 10  | C32   | 400  | PRO  | C-N   | 5.19  | 1.40        | 1.33     |
| 6   | O8    | 207  | ASP  | C-N   | -5.19 | 1.26        | 1.34     |
| 10  | C     | 549  | TYR  | C-N   | -5.19 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 1528 | PRO  | C-N   | 5.19  | 1.41        | 1.33     |
| 2   | M8    | 673  | ASN  | C-N   | 5.19  | 1.41        | 1.34     |
| 10  | C16   | 248  | LEU  | C-N   | 5.19  | 1.40        | 1.33     |
| 12  | A     | 782  | PRO  | C-N   | -5.19 | 1.26        | 1.33     |
| 13  | V     | 803  | GLN  | C-N   | -5.19 | 1.27        | 1.33     |
| 10  | C8    | 428  | GLY  | C-N   | 5.19  | 1.40        | 1.33     |
| 24  | D24   | 385  | PRO  | CA-C  | 5.19  | 1.54        | 1.51     |
| 18  | B     | 1239 | SER  | C-N   | 5.19  | 1.41        | 1.33     |
| 5   | P     | 61   | ASP  | C-N   | 5.18  | 1.40        | 1.33     |
| 5   | P8    | 128  | GLU  | C-N   | -5.18 | 1.26        | 1.33     |
| 10  | C24   | 428  | GLY  | C-N   | 5.18  | 1.40        | 1.33     |
| 10  | C     | 428  | GLY  | C-N   | 5.18  | 1.40        | 1.33     |
| 10  | C     | 452  | LEU  | C-N   | 5.18  | 1.40        | 1.33     |
| 18  | B     | 268  | GLN  | C-N   | -5.18 | 1.27        | 1.33     |
| 5   | P8    | 159  | ILE  | C-N   | -5.18 | 1.26        | 1.33     |
| 9   | K8    | 885  | ALA  | C-N   | -5.18 | 1.26        | 1.34     |
| 10  | C24   | 746  | GLY  | C-N   | -5.18 | 1.26        | 1.33     |
| 20  | E     | 260  | ASN  | C-N   | -5.18 | 1.27        | 1.34     |
| 23  | J32   | 584  | ARG  | C-N   | -5.18 | 1.27        | 1.33     |
| 10  | C24   | 785  | LEU  | C-N   | -5.18 | 1.27        | 1.33     |
| 2   | M     | 384  | ASP  | C-N   | 5.18  | 1.42        | 1.33     |
| 5   | P     | 159  | ILE  | C-N   | -5.18 | 1.26        | 1.33     |
| 5   | P16   | 615  | HIS  | C-N   | -5.18 | 1.26        | 1.33     |
| 10  | C16   | 634  | SER  | C-N   | -5.18 | 1.26        | 1.33     |
| 10  | C32   | 634  | SER  | C-N   | -5.18 | 1.26        | 1.33     |
| 3   | N     | 299  | ALA  | C-N   | 5.18  | 1.41        | 1.33     |
| 10  | C16   | 1138 | GLU  | C-N   | 5.18  | 1.41        | 1.33     |
| 10  | C16   | 1602 | GLY  | C-N   | 5.18  | 1.40        | 1.33     |
| 12  | A     | 851  | ARG  | C-N   | -5.18 | 1.26        | 1.34     |
| 10  | C     | 634  | SER  | C-N   | -5.18 | 1.26        | 1.33     |
| 18  | B8    | 268  | GLN  | C-N   | -5.18 | 1.27        | 1.33     |
| 18  | B8    | 1390 | LEU  | C-N   | 5.18  | 1.41        | 1.33     |
| 10  | C16   | 428  | GLY  | C-N   | 5.17  | 1.40        | 1.33     |
| 11  | A24   | 782  | PRO  | C-N   | -5.17 | 1.26        | 1.33     |
| 11  | A40   | 791  | PRO  | C-N   | 5.17  | 1.40        | 1.33     |
| 10  | C8    | 708  | GLN  | C-N   | -5.17 | 1.27        | 1.34     |
| 10  | C8    | 1756 | LEU  | C-N   | -5.17 | 1.26        | 1.33     |
| 10  | C8    | 93   | ASP  | C-N   | -5.17 | 1.26        | 1.33     |
| 10  | C8    | 698  | PHE  | C-N   | -5.17 | 1.27        | 1.33     |
| 18  | B8    | 285  | LEU  | C-N   | -5.17 | 1.26        | 1.34     |
| 10  | C32   | 708  | GLN  | C-N   | -5.17 | 1.27        | 1.34     |
| 2   | M     | 825  | THR  | C-N   | -5.17 | 1.27        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 7   | Q     | 263  | PRO  | N-CD  | 5.17  | 1.54        | 1.47     |
| 10  | C16   | 591  | ALA  | C-N   | 5.17  | 1.40        | 1.33     |
| 10  | C24   | 1756 | LEU  | C-N   | -5.17 | 1.27        | 1.33     |
| 10  | C     | 1695 | LEU  | C-N   | -5.17 | 1.27        | 1.33     |
| 18  | B     | 1164 | GLU  | C-N   | -5.17 | 1.26        | 1.34     |
| 22  | I24   | 321  | LYS  | C-N   | -5.17 | 1.27        | 1.34     |
| 23  | J24   | 606  | ILE  | C-N   | -5.17 | 1.27        | 1.33     |
| 5   | P8    | 444  | LEU  | C-N   | -5.17 | 1.27        | 1.33     |
| 10  | C24   | 708  | GLN  | C-N   | -5.17 | 1.27        | 1.34     |
| 10  | C24   | 1657 | SER  | C-N   | -5.17 | 1.26        | 1.33     |
| 12  | A     | 791  | PRO  | C-N   | 5.17  | 1.40        | 1.33     |
| 10  | C     | 93   | ASP  | C-N   | -5.17 | 1.26        | 1.33     |
| 10  | C     | 708  | GLN  | C-N   | -5.17 | 1.27        | 1.34     |
| 10  | C8    | 452  | LEU  | C-N   | 5.17  | 1.40        | 1.33     |
| 10  | C     | 523  | LYS  | C-N   | -5.17 | 1.26        | 1.33     |
| 10  | C     | 788  | LEU  | C-N   | -5.17 | 1.27        | 1.33     |
| 10  | C24   | 987  | TYR  | C-N   | 5.17  | 1.41        | 1.33     |
| 2   | M     | 337  | ASP  | C-N   | 5.16  | 1.40        | 1.33     |
| 2   | M     | 801  | GLU  | C-N   | -5.16 | 1.27        | 1.33     |
| 1   | R16   | 1249 | SER  | C-N   | -5.16 | 1.26        | 1.33     |
| 2   | M16   | 266  | PHE  | C-N   | -5.16 | 1.25        | 1.33     |
| 5   | P16   | 639  | THR  | C-N   | -5.16 | 1.26        | 1.33     |
| 10  | C     | 1284 | ASP  | C-N   | -5.16 | 1.27        | 1.33     |
| 18  | B8    | 1813 | SER  | C-N   | 5.16  | 1.41        | 1.33     |
| 10  | C24   | 1359 | ILE  | C-N   | -5.16 | 1.26        | 1.34     |
| 10  | C32   | 591  | ALA  | C-N   | 5.16  | 1.40        | 1.33     |
| 6   | O8    | 141  | PRO  | C-N   | -5.16 | 1.26        | 1.33     |
| 10  | C     | 1685 | SER  | C-N   | -5.16 | 1.27        | 1.33     |
| 10  | C8    | 523  | LYS  | C-N   | -5.16 | 1.26        | 1.33     |
| 18  | B8    | 727  | GLY  | C-N   | 5.16  | 1.40        | 1.33     |
| 10  | C16   | 400  | PRO  | C-N   | 5.16  | 1.40        | 1.33     |
| 10  | C8    | 1284 | ASP  | C-N   | -5.16 | 1.27        | 1.33     |
| 22  | I16   | 162  | GLN  | C-N   | -5.16 | 1.26        | 1.33     |
| 24  | D16   | 385  | PRO  | CA-C  | 5.16  | 1.54        | 1.51     |
| 10  | C16   | 770  | SER  | C-N   | 5.16  | 1.41        | 1.33     |
| 10  | C16   | 1743 | GLN  | C-N   | -5.16 | 1.27        | 1.33     |
| 10  | C8    | 400  | PRO  | C-N   | 5.16  | 1.40        | 1.33     |
| 18  | B     | 1910 | GLU  | C-N   | -5.16 | 1.27        | 1.33     |
| 18  | B8    | 1731 | PHE  | C-N   | -5.16 | 1.27        | 1.33     |
| 9   | K     | 1155 | THR  | C-N   | 5.15  | 1.40        | 1.33     |
| 1   | R8    | 1362 | ASP  | C-N   | -5.15 | 1.26        | 1.33     |
| 1   | R16   | 1362 | ASP  | C-N   | -5.15 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | P     | 413  | VAL  | C-N   | -5.15 | 1.27        | 1.33     |
| 5   | P     | 646  | PRO  | C-N   | -5.15 | 1.27        | 1.33     |
| 10  | C16   | 1685 | SER  | C-N   | -5.15 | 1.27        | 1.33     |
| 10  | C     | 746  | GLY  | C-N   | -5.15 | 1.26        | 1.33     |
| 10  | C8    | 1138 | GLU  | C-N   | 5.15  | 1.41        | 1.33     |
| 12  | A48   | 360  | GLU  | C-N   | -5.15 | 1.27        | 1.33     |
| 2   | M8    | 384  | ASP  | C-N   | 5.15  | 1.42        | 1.33     |
| 2   | M8    | 841  | GLN  | C-N   | -5.15 | 1.26        | 1.33     |
| 2   | M16   | 841  | GLN  | C-N   | -5.15 | 1.26        | 1.33     |
| 18  | B8    | 464  | ALA  | C-N   | 5.15  | 1.41        | 1.33     |
| 23  | J32   | 690  | ASP  | C-N   | -5.15 | 1.27        | 1.33     |
| 10  | C32   | 1602 | GLY  | C-N   | 5.15  | 1.40        | 1.33     |
| 20  | E8    | 371  | ALA  | C-N   | -5.15 | 1.26        | 1.33     |
| 2   | M16   | 825  | THR  | C-N   | -5.15 | 1.27        | 1.34     |
| 5   | P8    | 639  | THR  | C-N   | -5.15 | 1.26        | 1.33     |
| 10  | C24   | 575  | PHE  | C-N   | -5.15 | 1.25        | 1.33     |
| 10  | C     | 248  | LEU  | C-N   | 5.15  | 1.40        | 1.33     |
| 2   | M16   | 627  | TYR  | C-N   | -5.15 | 1.27        | 1.33     |
| 12  | A48   | 851  | ARG  | C-N   | -5.15 | 1.26        | 1.34     |
| 2   | M     | 340  | GLU  | C-N   | -5.14 | 1.26        | 1.33     |
| 7   | Q     | 33   | ARG  | C-N   | 5.14  | 1.41        | 1.33     |
| 7   | Q     | 179  | LEU  | C-N   | 5.14  | 1.41        | 1.33     |
| 10  | C8    | 1298 | SER  | C-N   | -5.14 | 1.27        | 1.33     |
| 2   | M8    | 627  | TYR  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C16   | 1633 | SER  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C16   | 1662 | ASP  | C-N   | 5.14  | 1.40        | 1.33     |
| 10  | C24   | 634  | SER  | C-N   | -5.14 | 1.26        | 1.33     |
| 10  | C24   | 1628 | SER  | C-N   | 5.14  | 1.41        | 1.33     |
| 14  | W     | 697  | ARG  | C-N   | -5.14 | 1.26        | 1.34     |
| 11  | A16   | 851  | ARG  | C-N   | -5.14 | 1.26        | 1.34     |
| 20  | E     | 371  | ALA  | C-N   | -5.14 | 1.26        | 1.33     |
| 22  | I8    | 162  | GLN  | C-N   | -5.14 | 1.26        | 1.33     |
| 23  | J16   | 606  | ILE  | C-N   | -5.14 | 1.27        | 1.33     |
| 5   | P16   | 444  | LEU  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C16   | 1284 | ASP  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C24   | 93   | ASP  | C-N   | -5.14 | 1.26        | 1.33     |
| 11  | A16   | 747  | MET  | C-N   | -5.14 | 1.27        | 1.33     |
| 2   | M8    | 340  | GLU  | C-N   | -5.14 | 1.26        | 1.33     |
| 5   | P     | 606  | ASP  | C-N   | -5.14 | 1.26        | 1.33     |
| 9   | K     | 916  | LYS  | C-N   | -5.14 | 1.26        | 1.33     |
| 10  | C24   | 418  | ASN  | C-N   | 5.14  | 1.40        | 1.34     |
| 11  | A32   | 782  | PRO  | C-N   | -5.14 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 18  | B     | 285  | LEU  | C-N   | -5.14 | 1.26        | 1.34     |
| 18  | B8    | 1362 | ALA  | C-N   | 5.14  | 1.40        | 1.33     |
| 20  | E     | 463  | ASP  | C-N   | -5.14 | 1.27        | 1.33     |
| 22  | I     | 321  | LYS  | C-N   | -5.14 | 1.27        | 1.34     |
| 10  | C32   | 1187 | GLY  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C32   | 1695 | LEU  | C-N   | -5.14 | 1.27        | 1.33     |
| 18  | B     | 1859 | LEU  | C-N   | -5.14 | 1.26        | 1.33     |
| 5   | P8    | 125  | ALA  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C24   | 378  | GLU  | C-N   | -5.14 | 1.27        | 1.33     |
| 11  | A40   | 625  | THR  | C-N   | -5.14 | 1.27        | 1.33     |
| 12  | A     | 747  | MET  | C-N   | -5.14 | 1.27        | 1.33     |
| 11  | A16   | 782  | PRO  | C-N   | -5.14 | 1.26        | 1.33     |
| 19  | 4     | 378  | TYR  | C-N   | -5.14 | 1.26        | 1.33     |
| 22  | I     | 202  | LEU  | C-N   | -5.14 | 1.26        | 1.33     |
| 23  | J16   | 584  | ARG  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C32   | 698  | PHE  | C-N   | -5.14 | 1.27        | 1.33     |
| 10  | C32   | 1298 | SER  | C-N   | -5.14 | 1.27        | 1.33     |
| 2   | M8    | 337  | ASP  | C-N   | 5.13  | 1.40        | 1.33     |
| 5   | P16   | 125  | ALA  | C-N   | -5.13 | 1.27        | 1.33     |
| 5   | P16   | 128  | GLU  | C-N   | -5.13 | 1.26        | 1.33     |
| 18  | B     | 207  | THR  | C-N   | -5.13 | 1.26        | 1.33     |
| 20  | E8    | 338  | GLU  | C-N   | 5.13  | 1.40        | 1.33     |
| 2   | M16   | 525  | ALA  | C-N   | 5.13  | 1.41        | 1.33     |
| 7   | Q8    | 263  | PRO  | N-CD  | 5.13  | 1.54        | 1.47     |
| 11  | A24   | 360  | GLU  | C-N   | -5.13 | 1.27        | 1.33     |
| 10  | C     | 271  | PHE  | C-N   | -5.13 | 1.27        | 1.33     |
| 10  | C     | 1602 | GLY  | C-N   | 5.13  | 1.40        | 1.33     |
| 20  | E8    | 171  | PHE  | C-N   | -5.13 | 1.26        | 1.33     |
| 20  | E8    | 463  | ASP  | C-N   | -5.13 | 1.27        | 1.33     |
| 7   | Q8    | 179  | LEU  | C-N   | 5.13  | 1.41        | 1.33     |
| 10  | C     | 1187 | GLY  | C-N   | -5.13 | 1.27        | 1.33     |
| 10  | C     | 1674 | LEU  | C-N   | -5.13 | 1.27        | 1.33     |
| 18  | B8    | 1289 | ASP  | C-N   | 5.13  | 1.40        | 1.33     |
| 10  | C16   | 271  | PHE  | C-N   | -5.13 | 1.27        | 1.33     |
| 10  | C16   | 708  | GLN  | C-N   | -5.13 | 1.27        | 1.34     |
| 10  | C16   | 1102 | SER  | C-N   | -5.13 | 1.26        | 1.33     |
| 10  | C16   | 1674 | LEU  | C-N   | -5.13 | 1.27        | 1.33     |
| 10  | C16   | 1695 | LEU  | C-N   | -5.13 | 1.27        | 1.33     |
| 18  | B     | 1590 | LEU  | C-N   | 5.13  | 1.40        | 1.33     |
| 18  | B8    | 391  | ARG  | C-N   | -5.13 | 1.27        | 1.34     |
| 20  | E     | 171  | PHE  | C-N   | -5.13 | 1.26        | 1.33     |
| 23  | J16   | 641  | ALA  | C-N   | -5.13 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | R8    | 1325 | GLN  | C-N   | -5.13 | 1.27        | 1.33     |
| 2   | M16   | 337  | ASP  | C-N   | 5.13  | 1.40        | 1.33     |
| 2   | M16   | 741  | SER  | C-N   | -5.13 | 1.27        | 1.33     |
| 5   | P     | 526  | ALA  | C-N   | -5.13 | 1.26        | 1.33     |
| 10  | C16   | 1657 | SER  | C-N   | -5.13 | 1.26        | 1.33     |
| 12  | A     | 551  | SER  | C-N   | -5.13 | 1.26        | 1.33     |
| 10  | C     | 698  | PHE  | C-N   | -5.13 | 1.27        | 1.33     |
| 19  | 48    | 378  | TYR  | C-N   | -5.13 | 1.26        | 1.33     |
| 23  | J24   | 584  | ARG  | C-N   | -5.13 | 1.27        | 1.33     |
| 1   | R     | 1362 | ASP  | C-N   | -5.12 | 1.27        | 1.33     |
| 5   | P     | 120  | SER  | C-N   | -5.12 | 1.26        | 1.33     |
| 7   | Q8    | 220  | ASN  | C-N   | 5.12  | 1.41        | 1.33     |
| 9   | K     | 585  | GLU  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C     | 1039 | ALA  | C-N   | -5.12 | 1.26        | 1.33     |
| 2   | M     | 407  | VAL  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C24   | 1695 | LEU  | C-N   | -5.12 | 1.27        | 1.33     |
| 18  | B8    | 1865 | LEU  | C-N   | 5.12  | 1.40        | 1.33     |
| 19  | 48    | 243  | SER  | C-N   | -5.12 | 1.26        | 1.33     |
| 23  | J32   | 641  | ALA  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C32   | 1628 | SER  | C-N   | 5.12  | 1.41        | 1.33     |
| 2   | M8    | 285  | ARG  | C-N   | -5.12 | 1.27        | 1.33     |
| 10  | C32   | 575  | PHE  | C-N   | -5.12 | 1.25        | 1.33     |
| 2   | M16   | 384  | ASP  | C-N   | 5.12  | 1.42        | 1.33     |
| 5   | P8    | 526  | ALA  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C16   | 788  | LEU  | C-N   | -5.12 | 1.27        | 1.33     |
| 10  | C8    | 1628 | SER  | C-N   | 5.12  | 1.41        | 1.33     |
| 10  | C32   | 746  | GLY  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C24   | 1284 | ASP  | C-N   | -5.12 | 1.27        | 1.33     |
| 10  | C24   | 1721 | GLN  | C-N   | 5.12  | 1.41        | 1.33     |
| 10  | C     | 1743 | GLN  | C-N   | -5.12 | 1.27        | 1.33     |
| 10  | C32   | 1662 | ASP  | C-N   | 5.12  | 1.40        | 1.33     |
| 5   | P     | 487  | GLU  | C-N   | -5.12 | 1.26        | 1.33     |
| 10  | C16   | 698  | PHE  | C-N   | -5.12 | 1.27        | 1.33     |
| 10  | C     | 1186 | TRP  | C-N   | 5.12  | 1.40        | 1.33     |
| 10  | C32   | 770  | SER  | C-N   | 5.12  | 1.40        | 1.33     |
| 2   | M     | 627  | TYR  | C-N   | -5.11 | 1.27        | 1.33     |
| 2   | M     | 841  | GLN  | C-N   | -5.11 | 1.26        | 1.33     |
| 1   | R8    | 1249 | SER  | C-N   | -5.11 | 1.26        | 1.33     |
| 6   | O     | 141  | PRO  | C-N   | -5.11 | 1.26        | 1.33     |
| 7   | Q8    | 89   | GLY  | C-N   | -5.11 | 1.26        | 1.33     |
| 10  | C     | 1138 | GLU  | C-N   | 5.11  | 1.40        | 1.33     |
| 10  | C8    | 122  | LEU  | C-N   | 5.11  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C8    | 1186 | TRP  | C-N   | 5.11  | 1.40        | 1.33     |
| 18  | B     | 391  | ARG  | C-N   | -5.11 | 1.27        | 1.34     |
| 20  | E     | 338  | GLU  | C-N   | 5.11  | 1.40        | 1.33     |
| 5   | P8    | 61   | ASP  | C-N   | 5.11  | 1.40        | 1.33     |
| 7   | Q16   | 33   | ARG  | C-N   | 5.11  | 1.40        | 1.33     |
| 10  | C     | 1662 | ASP  | C-N   | 5.11  | 1.40        | 1.33     |
| 18  | B8    | 733  | VAL  | C-N   | -5.11 | 1.27        | 1.33     |
| 9   | K     | 959  | TRP  | C-N   | -5.11 | 1.27        | 1.33     |
| 14  | W     | 755  | VAL  | C-N   | 5.11  | 1.41        | 1.33     |
| 10  | C8    | 1102 | SER  | C-N   | -5.11 | 1.26        | 1.33     |
| 18  | B     | 1813 | SER  | C-N   | 5.11  | 1.40        | 1.33     |
| 18  | B8    | 1239 | SER  | C-N   | 5.11  | 1.40        | 1.33     |
| 2   | M8    | 858  | SER  | C-N   | 5.11  | 1.40        | 1.33     |
| 10  | C16   | 575  | PHE  | C-N   | -5.11 | 1.25        | 1.33     |
| 10  | C24   | 452  | LEU  | C-N   | 5.11  | 1.40        | 1.33     |
| 18  | B     | 1417 | SER  | C-N   | 5.11  | 1.40        | 1.33     |
| 20  | E8    | 369  | TRP  | C-N   | -5.11 | 1.26        | 1.33     |
| 7   | Q8    | 74   | TRP  | C-N   | 5.11  | 1.40        | 1.33     |
| 11  | A32   | 298  | THR  | C-N   | 5.11  | 1.40        | 1.33     |
| 11  | A32   | 625  | THR  | C-N   | -5.11 | 1.27        | 1.33     |
| 11  | A32   | 747  | MET  | C-N   | -5.11 | 1.27        | 1.33     |
| 11  | A32   | 751  | THR  | C-N   | -5.11 | 1.27        | 1.33     |
| 18  | B8    | 207  | THR  | C-N   | -5.11 | 1.26        | 1.33     |
| 23  | J32   | 659  | GLU  | C-N   | -5.11 | 1.26        | 1.33     |
| 11  | A24   | 751  | THR  | C-N   | -5.11 | 1.27        | 1.33     |
| 11  | A40   | 747  | MET  | C-N   | -5.11 | 1.27        | 1.33     |
| 10  | C8    | 271  | PHE  | C-N   | -5.11 | 1.27        | 1.33     |
| 10  | C8    | 549  | TYR  | C-N   | -5.11 | 1.26        | 1.33     |
| 11  | A16   | 298  | THR  | C-N   | 5.11  | 1.40        | 1.33     |
| 10  | C32   | 1039 | ALA  | C-N   | -5.11 | 1.26        | 1.33     |
| 10  | C32   | 1680 | SER  | C-N   | -5.11 | 1.27        | 1.33     |
| 12  | A48   | 551  | SER  | C-N   | -5.11 | 1.26        | 1.33     |
| 9   | K8    | 714  | ARG  | C-N   | -5.10 | 1.27        | 1.33     |
| 10  | C     | 1721 | GLN  | C-N   | 5.10  | 1.41        | 1.33     |
| 18  | B     | 1730 | ALA  | C-N   | -5.10 | 1.27        | 1.33     |
| 2   | M8    | 407  | VAL  | C-N   | -5.10 | 1.26        | 1.33     |
| 7   | Q16   | 189  | SER  | C-N   | -5.10 | 1.27        | 1.33     |
| 9   | K8    | 826  | LEU  | C-N   | 5.10  | 1.37        | 1.33     |
| 10  | C     | 1359 | ILE  | C-N   | -5.10 | 1.26        | 1.34     |
| 10  | C8    | 248  | LEU  | C-N   | 5.10  | 1.40        | 1.33     |
| 10  | C8    | 1039 | ALA  | C-N   | -5.10 | 1.26        | 1.33     |
| 10  | C32   | 808  | PRO  | C-N   | -5.10 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C24   | 332  | SER  | C-N   | 5.10  | 1.40        | 1.34     |
| 10  | C24   | 1602 | GLY  | C-N   | 5.10  | 1.40        | 1.33     |
| 19  | 48    | 48   | ASP  | C-N   | -5.10 | 1.25        | 1.33     |
| 1   | R     | 1249 | SER  | C-N   | -5.10 | 1.26        | 1.33     |
| 6   | O8    | 30   | ASN  | C-N   | -5.10 | 1.26        | 1.33     |
| 7   | Q8    | 33   | ARG  | C-N   | 5.10  | 1.40        | 1.33     |
| 9   | K8    | 872  | THR  | C-N   | -5.10 | 1.27        | 1.33     |
| 10  | C16   | 378  | GLU  | C-N   | -5.10 | 1.27        | 1.33     |
| 10  | C8    | 759  | VAL  | C-N   | -5.10 | 1.25        | 1.32     |
| 11  | A16   | 551  | SER  | C-N   | -5.10 | 1.26        | 1.33     |
| 18  | B     | 1144 | LYS  | C-N   | 5.10  | 1.41        | 1.33     |
| 19  | 4     | 243  | SER  | C-N   | -5.10 | 1.26        | 1.33     |
| 10  | C32   | 1483 | GLY  | C-N   | 5.10  | 1.40        | 1.33     |
| 7   | Q     | 74   | TRP  | C-N   | 5.10  | 1.40        | 1.33     |
| 7   | Q16   | 263  | PRO  | N-CD  | 5.10  | 1.54        | 1.47     |
| 12  | A     | 553  | THR  | C-N   | -5.10 | 1.26        | 1.33     |
| 10  | C32   | 1102 | SER  | C-N   | -5.10 | 1.26        | 1.33     |
| 10  | C24   | 759  | VAL  | C-N   | -5.10 | 1.25        | 1.32     |
| 10  | C8    | 1633 | SER  | C-N   | -5.10 | 1.27        | 1.33     |
| 10  | C24   | 591  | ALA  | C-N   | 5.09  | 1.40        | 1.33     |
| 2   | M16   | 407  | VAL  | C-N   | -5.09 | 1.27        | 1.33     |
| 3   | N16   | 43   | ASN  | C-N   | 5.09  | 1.41        | 1.33     |
| 6   | O     | 30   | ASN  | C-N   | -5.09 | 1.26        | 1.33     |
| 9   | K8    | 1155 | THR  | C-N   | 5.09  | 1.40        | 1.33     |
| 10  | C8    | 1674 | LEU  | C-N   | -5.09 | 1.27        | 1.33     |
| 11  | A32   | 851  | ARG  | C-N   | -5.09 | 1.26        | 1.34     |
| 24  | D40   | 385  | PRO  | CA-C  | 5.09  | 1.54        | 1.51     |
| 12  | A48   | 747  | MET  | C-N   | -5.09 | 1.27        | 1.33     |
| 3   | N8    | 43   | ASN  | C-N   | 5.09  | 1.41        | 1.33     |
| 7   | Q     | 220  | ASN  | C-N   | 5.09  | 1.40        | 1.33     |
| 5   | P8    | 487  | GLU  | C-N   | -5.09 | 1.26        | 1.33     |
| 6   | O16   | 30   | ASN  | C-N   | -5.09 | 1.26        | 1.33     |
| 10  | C16   | 1039 | ALA  | C-N   | -5.09 | 1.27        | 1.33     |
| 10  | C24   | 1633 | SER  | C-N   | -5.09 | 1.27        | 1.33     |
| 18  | B8    | 1273 | GLU  | C-N   | 5.09  | 1.40        | 1.33     |
| 22  | I16   | 321  | LYS  | C-N   | -5.09 | 1.27        | 1.34     |
| 6   | O16   | 10   | SER  | C-N   | -5.09 | 1.26        | 1.33     |
| 10  | C24   | 788  | LEU  | C-N   | -5.09 | 1.27        | 1.33     |
| 10  | C     | 1483 | GLY  | C-N   | 5.09  | 1.40        | 1.33     |
| 11  | A16   | 751  | THR  | C-N   | -5.09 | 1.27        | 1.33     |
| 23  | J8    | 690  | ASP  | C-N   | -5.09 | 1.27        | 1.33     |
| 10  | C32   | 1743 | GLN  | C-N   | -5.09 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M8    | 525  | ALA  | C-N   | 5.09  | 1.41        | 1.33     |
| 10  | C16   | 1037 | SER  | C-N   | -5.09 | 1.26        | 1.33     |
| 22  | I24   | 202  | LEU  | C-N   | -5.09 | 1.26        | 1.33     |
| 7   | Q16   | 179  | LEU  | C-N   | 5.09  | 1.41        | 1.33     |
| 9   | K     | 628  | LYS  | C-N   | -5.09 | 1.26        | 1.34     |
| 11  | A24   | 851  | ARG  | C-N   | -5.09 | 1.26        | 1.34     |
| 23  | J24   | 641  | ALA  | C-N   | -5.09 | 1.27        | 1.33     |
| 10  | C24   | 1039 | ALA  | C-N   | -5.08 | 1.27        | 1.33     |
| 11  | A40   | 751  | THR  | C-N   | -5.08 | 1.27        | 1.33     |
| 5   | P8    | 413  | VAL  | C-N   | -5.08 | 1.27        | 1.33     |
| 6   | O16   | 141  | PRO  | C-N   | -5.08 | 1.26        | 1.33     |
| 10  | C16   | 1187 | GLY  | C-N   | -5.08 | 1.27        | 1.33     |
| 10  | C16   | 1628 | SER  | C-N   | 5.08  | 1.41        | 1.33     |
| 10  | C8    | 1680 | SER  | C-N   | -5.08 | 1.27        | 1.33     |
| 18  | B8    | 165  | GLU  | C-N   | -5.08 | 1.27        | 1.33     |
| 9   | K8    | 620  | ALA  | C-N   | 5.08  | 1.40        | 1.33     |
| 11  | A24   | 298  | THR  | C-N   | 5.08  | 1.40        | 1.33     |
| 10  | C24   | 800  | ASP  | C-N   | 5.08  | 1.40        | 1.33     |
| 10  | C     | 1680 | SER  | C-N   | -5.08 | 1.27        | 1.33     |
| 23  | J16   | 549  | GLU  | C-N   | -5.08 | 1.27        | 1.33     |
| 15  | J     | 576  | LEU  | C-N   | -5.08 | 1.27        | 1.33     |
| 23  | J16   | 659  | GLU  | C-N   | -5.08 | 1.27        | 1.33     |
| 10  | C32   | 1193 | ASN  | C-N   | -5.08 | 1.27        | 1.33     |
| 5   | P     | 39   | LEU  | C-N   | -5.08 | 1.25        | 1.33     |
| 6   | O8    | 10   | SER  | C-N   | -5.08 | 1.26        | 1.33     |
| 11  | A24   | 625  | THR  | C-N   | -5.08 | 1.27        | 1.33     |
| 10  | C     | 1628 | SER  | C-N   | 5.08  | 1.41        | 1.33     |
| 10  | C32   | 1284 | ASP  | C-N   | -5.08 | 1.27        | 1.33     |
| 7   | Q     | 89   | GLY  | C-N   | -5.08 | 1.26        | 1.33     |
| 18  | B     | 1731 | PHE  | C-N   | -5.08 | 1.27        | 1.33     |
| 10  | C32   | 387  | ALA  | C-N   | -5.08 | 1.26        | 1.33     |
| 10  | C32   | 759  | VAL  | C-N   | -5.08 | 1.25        | 1.32     |
| 5   | P     | 639  | THR  | C-N   | -5.08 | 1.27        | 1.33     |
| 7   | Q8    | 210  | SER  | C-N   | 5.08  | 1.39        | 1.33     |
| 10  | C16   | 759  | VAL  | C-N   | -5.08 | 1.25        | 1.32     |
| 18  | B     | 1180 | VAL  | C-N   | -5.08 | 1.27        | 1.33     |
| 18  | B     | 1362 | ALA  | C-N   | 5.08  | 1.40        | 1.33     |
| 2   | M16   | 422  | LEU  | C-N   | -5.07 | 1.26        | 1.33     |
| 9   | K8    | 628  | LYS  | C-N   | -5.07 | 1.26        | 1.34     |
| 15  | J     | 604  | GLU  | C-N   | -5.07 | 1.27        | 1.33     |
| 10  | C     | 400  | PRO  | C-N   | 5.07  | 1.40        | 1.33     |
| 18  | B     | 733  | VAL  | C-N   | -5.07 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | I8    | 321  | LYS  | C-N   | -5.07 | 1.27        | 1.34     |
| 2   | M     | 525  | ALA  | C-N   | 5.07  | 1.41        | 1.33     |
| 7   | Q16   | 265  | VAL  | C-N   | -5.07 | 1.26        | 1.33     |
| 23  | J16   | 629  | ASN  | C-N   | 5.07  | 1.41        | 1.34     |
| 5   | P16   | 608  | LYS  | C-N   | -5.07 | 1.27        | 1.33     |
| 9   | K     | 620  | ALA  | C-N   | 5.07  | 1.40        | 1.33     |
| 11  | A24   | 551  | SER  | C-N   | -5.07 | 1.26        | 1.33     |
| 11  | A24   | 553  | THR  | C-N   | -5.07 | 1.26        | 1.33     |
| 11  | A40   | 551  | SER  | C-N   | -5.07 | 1.26        | 1.33     |
| 20  | E8    | 284  | LEU  | C-N   | -5.07 | 1.27        | 1.33     |
| 10  | C32   | 987  | TYR  | C-N   | 5.07  | 1.40        | 1.33     |
| 12  | A48   | 147  | PHE  | C-N   | 5.07  | 1.41        | 1.34     |
| 10  | C24   | 1674 | LEU  | C-N   | -5.07 | 1.27        | 1.33     |
| 18  | B     | 652  | LEU  | C-N   | -5.07 | 1.27        | 1.34     |
| 10  | C32   | 1633 | SER  | C-N   | -5.07 | 1.27        | 1.33     |
| 10  | C32   | 1657 | SER  | C-N   | -5.07 | 1.26        | 1.33     |
| 2   | M16   | 527  | GLY  | C-N   | -5.07 | 1.26        | 1.33     |
| 10  | C8    | 1359 | ILE  | C-N   | -5.07 | 1.26        | 1.34     |
| 18  | B     | 1865 | LEU  | C-N   | 5.07  | 1.40        | 1.33     |
| 7   | Q     | 283  | GLU  | C-N   | -5.07 | 1.27        | 1.33     |
| 6   | O8    | 79   | ASP  | C-N   | -5.07 | 1.26        | 1.33     |
| 10  | C8    | 1193 | ASN  | C-N   | -5.07 | 1.27        | 1.33     |
| 11  | A16   | 337  | ARG  | C-N   | 5.07  | 1.41        | 1.33     |
| 18  | B8    | 85   | ASP  | C-N   | -5.07 | 1.27        | 1.33     |
| 22  | I16   | 202  | LEU  | C-N   | -5.07 | 1.26        | 1.33     |
| 10  | C32   | 986  | LYS  | C-N   | -5.07 | 1.26        | 1.33     |
| 7   | Q     | 63   | ASN  | C-N   | 5.06  | 1.40        | 1.33     |
| 7   | Q     | 210  | SER  | C-N   | 5.06  | 1.39        | 1.33     |
| 11  | A40   | 298  | THR  | C-N   | 5.06  | 1.40        | 1.33     |
| 18  | B     | 1635 | GLY  | C-N   | 5.06  | 1.41        | 1.33     |
| 23  | J8    | 549  | GLU  | C-N   | -5.06 | 1.27        | 1.33     |
| 10  | C32   | 271  | PHE  | C-N   | -5.06 | 1.27        | 1.33     |
| 9   | K     | 937  | ILE  | C-N   | -5.06 | 1.27        | 1.33     |
| 9   | K     | 1279 | GLU  | C-N   | -5.06 | 1.26        | 1.33     |
| 10  | C32   | 1571 | PHE  | C-N   | 5.06  | 1.41        | 1.33     |
| 5   | P16   | 526  | ALA  | C-N   | -5.06 | 1.27        | 1.33     |
| 9   | K8    | 717  | ARG  | C-N   | -5.06 | 1.26        | 1.33     |
| 10  | C16   | 1359 | ILE  | C-N   | -5.06 | 1.26        | 1.34     |
| 11  | A16   | 621  | LYS  | C-N   | -5.06 | 1.27        | 1.33     |
| 2   | M     | 285  | ARG  | C-N   | -5.06 | 1.27        | 1.33     |
| 7   | Q16   | 283  | GLU  | C-N   | -5.06 | 1.27        | 1.33     |
| 13  | V     | 740  | GLU  | C-N   | -5.06 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A32   | 551  | SER  | C-N   | -5.06 | 1.26        | 1.33     |
| 6   | O     | 79   | ASP  | C-N   | -5.05 | 1.26        | 1.33     |
| 10  | C16   | 122  | LEU  | C-N   | 5.05  | 1.40        | 1.33     |
| 10  | C16   | 987  | TYR  | C-N   | 5.05  | 1.40        | 1.33     |
| 10  | C16   | 1680 | SER  | C-N   | -5.05 | 1.27        | 1.33     |
| 10  | C24   | 1685 | SER  | C-N   | -5.05 | 1.27        | 1.33     |
| 10  | C     | 1785 | SER  | C-N   | -5.05 | 1.27        | 1.34     |
| 23  | J24   | 549  | GLU  | C-N   | -5.05 | 1.27        | 1.33     |
| 24  | D8    | 385  | PRO  | CA-C  | 5.05  | 1.54        | 1.51     |
| 10  | C24   | 122  | LEU  | C-N   | 5.05  | 1.40        | 1.33     |
| 18  | B8    | 652  | LEU  | C-N   | -5.05 | 1.27        | 1.34     |
| 20  | E     | 379  | SER  | C-N   | -5.05 | 1.27        | 1.33     |
| 10  | C32   | 122  | LEU  | C-N   | 5.05  | 1.40        | 1.33     |
| 10  | C16   | 332  | SER  | C-N   | 5.05  | 1.40        | 1.34     |
| 10  | C24   | 443  | SER  | C-N   | -5.05 | 1.27        | 1.33     |
| 11  | A32   | 677  | ASP  | C-N   | -5.05 | 1.27        | 1.33     |
| 20  | E     | 307  | THR  | C-N   | -5.05 | 1.26        | 1.33     |
| 23  | J8    | 641  | ALA  | C-N   | -5.05 | 1.27        | 1.33     |
| 22  | I24   | 162  | GLN  | C-N   | -5.05 | 1.27        | 1.33     |
| 24  | D     | 385  | PRO  | CA-C  | 5.05  | 1.54        | 1.51     |
| 2   | M     | 858  | SER  | C-N   | 5.05  | 1.40        | 1.33     |
| 6   | O     | 10   | SER  | C-N   | -5.05 | 1.26        | 1.33     |
| 5   | P16   | 487  | GLU  | C-N   | -5.05 | 1.26        | 1.33     |
| 10  | C     | 332  | SER  | C-N   | 5.05  | 1.40        | 1.34     |
| 11  | A32   | 337  | ARG  | C-N   | 5.05  | 1.41        | 1.33     |
| 22  | I     | 162  | GLN  | C-N   | -5.05 | 1.27        | 1.33     |
| 23  | J32   | 634  | SER  | C-N   | -5.05 | 1.27        | 1.33     |
| 5   | P     | 608  | LYS  | C-N   | -5.05 | 1.27        | 1.33     |
| 18  | B     | 165  | GLU  | C-N   | -5.05 | 1.27        | 1.33     |
| 18  | B8    | 1582 | PHE  | C-N   | 5.05  | 1.40        | 1.33     |
| 18  | B     | 187  | LEU  | C-N   | 5.04  | 1.41        | 1.33     |
| 19  | 4     | 48   | ASP  | C-N   | -5.04 | 1.25        | 1.33     |
| 23  | J8    | 629  | ASN  | C-N   | 5.04  | 1.41        | 1.34     |
| 9   | K     | 714  | ARG  | C-N   | -5.04 | 1.27        | 1.33     |
| 11  | A32   | 553  | THR  | C-N   | -5.04 | 1.26        | 1.33     |
| 1   | R8    | 1174 | GLY  | C-N   | 5.04  | 1.42        | 1.34     |
| 1   | R16   | 1174 | GLY  | C-N   | 5.04  | 1.42        | 1.34     |
| 9   | K8    | 959  | TRP  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C24   | 156  | GLN  | C-N   | 5.04  | 1.40        | 1.33     |
| 11  | A32   | 621  | LYS  | C-N   | -5.04 | 1.27        | 1.33     |
| 18  | B8    | 1180 | VAL  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C32   | 378  | GLU  | C-N   | -5.04 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | C32   | 443  | SER  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C16   | 986  | LYS  | C-N   | -5.04 | 1.26        | 1.33     |
| 10  | C     | 1170 | VAL  | C-N   | -5.04 | 1.27        | 1.33     |
| 18  | B     | 1582 | PHE  | C-N   | 5.04  | 1.40        | 1.33     |
| 18  | B8    | 1859 | LEU  | C-N   | -5.04 | 1.27        | 1.33     |
| 20  | E     | 369  | TRP  | C-N   | -5.04 | 1.27        | 1.33     |
| 23  | J32   | 549  | GLU  | C-N   | -5.04 | 1.27        | 1.33     |
| 2   | M16   | 285  | ARG  | C-N   | -5.04 | 1.27        | 1.33     |
| 5   | P8    | 120  | SER  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C16   | 1785 | SER  | C-N   | -5.04 | 1.27        | 1.34     |
| 10  | C24   | 387  | ALA  | C-N   | -5.04 | 1.26        | 1.33     |
| 10  | C24   | 1037 | SER  | C-N   | -5.04 | 1.26        | 1.33     |
| 10  | C24   | 1170 | VAL  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C24   | 1571 | PHE  | C-N   | 5.04  | 1.40        | 1.33     |
| 10  | C     | 443  | SER  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C     | 759  | VAL  | C-N   | -5.04 | 1.25        | 1.32     |
| 18  | B8    | 1730 | ALA  | C-N   | -5.04 | 1.27        | 1.33     |
| 22  | I     | 289  | LEU  | C-N   | -5.04 | 1.27        | 1.34     |
| 10  | C32   | 580  | GLY  | C-N   | 5.04  | 1.40        | 1.33     |
| 10  | C32   | 963  | GLN  | C-N   | 5.04  | 1.40        | 1.33     |
| 5   | P16   | 514  | GLU  | C-N   | -5.04 | 1.27        | 1.33     |
| 7   | Q16   | 63   | ASN  | C-N   | 5.04  | 1.40        | 1.33     |
| 7   | Q16   | 210  | SER  | C-N   | 5.04  | 1.39        | 1.33     |
| 10  | C24   | 580  | GLY  | C-N   | 5.04  | 1.40        | 1.33     |
| 10  | C24   | 1193 | ASN  | C-N   | -5.04 | 1.27        | 1.33     |
| 15  | J     | 555  | GLN  | C-N   | -5.04 | 1.27        | 1.33     |
| 10  | C     | 800  | ASP  | C-N   | 5.04  | 1.40        | 1.33     |
| 10  | C32   | 1215 | ALA  | C-N   | -5.04 | 1.26        | 1.33     |
| 9   | K8    | 901  | TRP  | C-N   | -5.03 | 1.27        | 1.33     |
| 18  | B     | 1273 | GLU  | C-N   | 5.03  | 1.40        | 1.33     |
| 10  | C32   | 1359 | ILE  | C-N   | -5.03 | 1.27        | 1.34     |
| 9   | K     | 872  | THR  | C-N   | -5.03 | 1.27        | 1.33     |
| 23  | J8    | 659  | GLU  | C-N   | -5.03 | 1.27        | 1.33     |
| 1   | R8    | 1190 | VAL  | C-N   | 5.03  | 1.40        | 1.33     |
| 7   | Q8    | 189  | SER  | C-N   | -5.03 | 1.27        | 1.33     |
| 5   | P16   | 39   | LEU  | C-N   | -5.03 | 1.25        | 1.33     |
| 5   | P16   | 45   | CYS  | C-N   | -5.03 | 1.26        | 1.33     |
| 7   | Q16   | 220  | ASN  | C-N   | 5.03  | 1.40        | 1.33     |
| 9   | K8    | 916  | LYS  | C-N   | -5.03 | 1.27        | 1.33     |
| 10  | C24   | 1215 | ALA  | C-N   | -5.03 | 1.26        | 1.33     |
| 18  | B8    | 1635 | GLY  | C-N   | 5.03  | 1.41        | 1.33     |
| 7   | Q16   | 74   | TRP  | C-N   | 5.03  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | K     | 803  | VAL  | C-N   | -5.03 | 1.27        | 1.33     |
| 10  | C     | 1056 | VAL  | C-N   | -5.03 | 1.27        | 1.33     |
| 10  | C     | 1571 | PHE  | C-N   | 5.03  | 1.40        | 1.33     |
| 10  | C8    | 1215 | ALA  | C-N   | -5.03 | 1.26        | 1.33     |
| 11  | A16   | 625  | THR  | C-N   | -5.03 | 1.27        | 1.33     |
| 18  | B     | 1289 | ASP  | C-N   | 5.03  | 1.40        | 1.33     |
| 10  | C32   | 800  | ASP  | C-N   | 5.03  | 1.40        | 1.33     |
| 1   | R16   | 1277 | LEU  | C-N   | -5.03 | 1.27        | 1.33     |
| 5   | P8    | 608  | LYS  | C-N   | -5.03 | 1.27        | 1.33     |
| 10  | C16   | 963  | GLN  | C-N   | 5.03  | 1.40        | 1.33     |
| 11  | A40   | 654  | PRO  | N-CD  | -5.03 | 1.40        | 1.47     |
| 15  | J     | 654  | VAL  | C-N   | -5.03 | 1.27        | 1.33     |
| 11  | A16   | 677  | ASP  | C-N   | -5.03 | 1.27        | 1.33     |
| 18  | B8    | 1417 | SER  | C-N   | 5.03  | 1.40        | 1.33     |
| 10  | C32   | 332  | SER  | C-N   | 5.03  | 1.40        | 1.34     |
| 12  | A48   | 553  | THR  | C-N   | -5.03 | 1.26        | 1.33     |
| 3   | N     | 16   | ASP  | C-N   | -5.02 | 1.26        | 1.33     |
| 7   | Q16   | 89   | GLY  | C-N   | -5.02 | 1.26        | 1.33     |
| 10  | C24   | 1483 | GLY  | C-N   | 5.02  | 1.40        | 1.33     |
| 23  | J32   | 629  | ASN  | C-N   | 5.02  | 1.40        | 1.34     |
| 2   | M     | 728  | GLU  | C-N   | -5.02 | 1.27        | 1.33     |
| 5   | P     | 514  | GLU  | C-N   | -5.02 | 1.27        | 1.33     |
| 10  | C16   | 156  | GLN  | C-N   | 5.02  | 1.40        | 1.33     |
| 1   | R     | 1174 | GLY  | C-N   | 5.02  | 1.42        | 1.34     |
| 10  | C16   | 1571 | PHE  | C-N   | 5.02  | 1.40        | 1.33     |
| 10  | C24   | 1056 | VAL  | C-N   | -5.02 | 1.27        | 1.33     |
| 14  | W     | 798  | VAL  | C-N   | -5.02 | 1.27        | 1.33     |
| 11  | A16   | 553  | THR  | C-N   | -5.02 | 1.26        | 1.33     |
| 3   | N     | 150  | PRO  | N-CD  | 5.02  | 1.54        | 1.47     |
| 2   | M16   | 858  | SER  | C-N   | 5.02  | 1.40        | 1.33     |
| 5   | P8    | 39   | LEU  | C-N   | -5.02 | 1.25        | 1.33     |
| 10  | C24   | 1680 | SER  | C-N   | -5.02 | 1.27        | 1.33     |
| 18  | B     | 1914 | VAL  | C-N   | -5.02 | 1.26        | 1.33     |
| 18  | B8    | 726  | GLU  | C-N   | 5.02  | 1.41        | 1.33     |
| 18  | B8    | 1144 | LYS  | C-N   | 5.02  | 1.41        | 1.33     |
| 12  | A48   | 625  | THR  | C-N   | -5.02 | 1.27        | 1.33     |
| 5   | P     | 323  | SER  | C-N   | -5.02 | 1.26        | 1.33     |
| 5   | P8    | 45   | CYS  | C-N   | -5.02 | 1.26        | 1.33     |
| 5   | P8    | 323  | SER  | C-N   | -5.02 | 1.26        | 1.33     |
| 5   | P16   | 323  | SER  | C-N   | -5.02 | 1.26        | 1.33     |
| 10  | C8    | 443  | SER  | C-N   | -5.02 | 1.27        | 1.33     |
| 10  | C8    | 1721 | GLN  | C-N   | 5.02  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 20  | E8    | 307  | THR  | C-N   | -5.02 | 1.26        | 1.33     |
| 22  | I8    | 289  | LEU  | C-N   | -5.02 | 1.27        | 1.34     |
| 12  | A48   | 751  | THR  | C-N   | -5.02 | 1.27        | 1.33     |
| 10  | C     | 1215 | ALA  | C-N   | -5.02 | 1.26        | 1.33     |
| 3   | N     | 43   | ASN  | C-N   | 5.01  | 1.41        | 1.33     |
| 5   | P8    | 514  | GLU  | C-N   | -5.01 | 1.27        | 1.33     |
| 7   | Q8    | 63   | ASN  | C-N   | 5.01  | 1.40        | 1.33     |
| 10  | C16   | 387  | ALA  | C-N   | -5.01 | 1.26        | 1.33     |
| 12  | A     | 625  | THR  | C-N   | -5.01 | 1.27        | 1.33     |
| 10  | C     | 387  | ALA  | C-N   | -5.01 | 1.26        | 1.33     |
| 18  | B8    | 600  | SER  | C-N   | 5.01  | 1.40        | 1.33     |
| 22  | I8    | 181  | LEU  | C-N   | -5.01 | 1.27        | 1.33     |
| 22  | I16   | 181  | LEU  | C-N   | -5.01 | 1.27        | 1.33     |
| 10  | C32   | 1685 | SER  | C-N   | -5.01 | 1.27        | 1.33     |
| 7   | Q     | 265  | VAL  | C-N   | -5.01 | 1.26        | 1.33     |
| 7   | Q16   | 185  | VAL  | C-N   | 5.01  | 1.40        | 1.33     |
| 10  | C24   | 1662 | ASP  | C-N   | 5.01  | 1.40        | 1.33     |
| 18  | B     | 675  | SER  | C-N   | 5.01  | 1.40        | 1.34     |
| 22  | I8    | 101  | ALA  | C-N   | -5.01 | 1.27        | 1.33     |
| 10  | C24   | 1112 | LEU  | C-N   | -5.01 | 1.26        | 1.33     |
| 13  | V     | 842  | HIS  | C-N   | -5.01 | 1.27        | 1.33     |
| 10  | C8    | 963  | GLN  | C-N   | 5.01  | 1.40        | 1.33     |
| 18  | B8    | 1589 | LEU  | C-N   | 5.01  | 1.41        | 1.33     |
| 22  | I16   | 289  | LEU  | C-N   | -5.01 | 1.27        | 1.34     |
| 5   | P     | 702  | LEU  | C-N   | -5.01 | 1.27        | 1.33     |
| 10  | C8    | 156  | GLN  | C-N   | 5.01  | 1.40        | 1.33     |
| 10  | C8    | 387  | ALA  | C-N   | -5.01 | 1.26        | 1.33     |
| 21  | H     | 358  | ARG  | C-N   | -5.01 | 1.27        | 1.33     |
| 22  | I8    | 202  | LEU  | C-N   | -5.01 | 1.26        | 1.33     |
| 23  | J24   | 690  | ASP  | C-N   | -5.01 | 1.27        | 1.33     |
| 1   | R     | 1263 | MET  | C-N   | -5.01 | 1.27        | 1.33     |
| 9   | K8    | 937  | ILE  | C-N   | -5.01 | 1.27        | 1.33     |
| 2   | M8    | 728  | GLU  | C-N   | -5.01 | 1.27        | 1.33     |
| 2   | M16   | 404  | ASP  | C-N   | -5.01 | 1.27        | 1.33     |
| 7   | Q     | 189  | SER  | C-N   | -5.01 | 1.27        | 1.33     |
| 5   | P8    | 702  | LEU  | C-N   | -5.01 | 1.27        | 1.33     |
| 22  | I     | 181  | LEU  | C-N   | -5.01 | 1.27        | 1.33     |
| 12  | A48   | 654  | PRO  | N-CD  | -5.01 | 1.40        | 1.47     |
| 23  | J24   | 629  | ASN  | C-N   | 5.00  | 1.40        | 1.34     |
| 10  | C32   | 156  | GLN  | C-N   | 5.00  | 1.40        | 1.33     |
| 10  | C32   | 1170 | VAL  | C-N   | -5.00 | 1.27        | 1.33     |
| 3   | N8    | 16   | ASP  | C-N   | -5.00 | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | M16   | 577  | HIS  | C-N   | -5.00 | 1.27        | 1.33     |
| 6   | O16   | 79   | ASP  | C-N   | -5.00 | 1.26        | 1.33     |
| 10  | C16   | 1483 | GLY  | C-N   | 5.00  | 1.40        | 1.33     |
| 13  | V     | 901  | THR  | C-N   | -5.00 | 1.27        | 1.33     |
| 10  | C     | 378  | GLU  | C-N   | -5.00 | 1.27        | 1.33     |
| 11  | A32   | 384  | THR  | C-N   | -5.00 | 1.26        | 1.33     |
| 19  | 4     | 309  | GLY  | C-N   | 5.00  | 1.41        | 1.33     |
| 23  | J16   | 634  | SER  | C-N   | -5.00 | 1.27        | 1.33     |
| 7   | Q     | 185  | VAL  | C-N   | 5.00  | 1.40        | 1.33     |
| 5   | P16   | 120  | SER  | C-N   | -5.00 | 1.27        | 1.33     |
| 9   | K8    | 1028 | GLN  | C-N   | -5.00 | 1.27        | 1.34     |
| 10  | C16   | 1193 | ASN  | C-N   | -5.00 | 1.27        | 1.33     |
| 12  | A     | 751  | THR  | C-N   | -5.00 | 1.27        | 1.33     |
| 19  | 48    | 309  | GLY  | C-N   | 5.00  | 1.41        | 1.33     |
| 23  | J8    | 590  | ALA  | C-N   | -5.00 | 1.27        | 1.33     |

All (6602) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 8   | L8    | 1054 | HIS  | ND1-CE1-NE2 | -53.29 | 55.11       | 108.40   |
| 8   | L     | 1054 | HIS  | ND1-CE1-NE2 | -53.27 | 55.12       | 108.40   |
| 8   | L16   | 1054 | HIS  | ND1-CE1-NE2 | -53.26 | 55.14       | 108.40   |
| 1   | R16   | 529  | HIS  | ND1-CE1-NE2 | -52.76 | 55.64       | 108.40   |
| 1   | R     | 529  | HIS  | ND1-CE1-NE2 | -52.75 | 55.65       | 108.40   |
| 1   | R8    | 529  | HIS  | ND1-CE1-NE2 | -52.74 | 55.66       | 108.40   |
| 4   | T     | 160  | HIS  | ND1-CE1-NE2 | -52.23 | 56.16       | 108.40   |
| 4   | T8    | 160  | HIS  | ND1-CE1-NE2 | -52.18 | 56.22       | 108.40   |
| 4   | T16   | 160  | HIS  | ND1-CE1-NE2 | -52.18 | 56.22       | 108.40   |
| 4   | T     | 160  | HIS  | CE1-NE2-CD2 | -44.26 | 64.74       | 109.00   |
| 4   | T8    | 160  | HIS  | CE1-NE2-CD2 | -44.23 | 64.77       | 109.00   |
| 4   | T16   | 160  | HIS  | CE1-NE2-CD2 | -44.21 | 64.79       | 109.00   |
| 8   | L8    | 1054 | HIS  | CE1-NE2-CD2 | -43.74 | 65.26       | 109.00   |
| 8   | L16   | 1054 | HIS  | CE1-NE2-CD2 | -43.72 | 65.28       | 109.00   |
| 8   | L     | 1054 | HIS  | CE1-NE2-CD2 | -43.69 | 65.31       | 109.00   |
| 1   | R     | 529  | HIS  | CE1-NE2-CD2 | -43.67 | 65.33       | 109.00   |
| 1   | R8    | 529  | HIS  | CE1-NE2-CD2 | -43.66 | 65.34       | 109.00   |
| 1   | R16   | 529  | HIS  | CE1-NE2-CD2 | -43.65 | 65.35       | 109.00   |
| 1   | R     | 1381 | GLU  | O-C-N       | -40.39 | 69.77       | 122.28   |
| 1   | R8    | 1381 | GLU  | O-C-N       | -40.38 | 69.78       | 122.28   |
| 1   | R16   | 1381 | GLU  | O-C-N       | -40.38 | 69.78       | 122.28   |
| 10  | C24   | 670  | GLU  | O-C-N       | -37.38 | 93.44       | 121.47   |
| 10  | C8    | 670  | GLU  | O-C-N       | -37.36 | 93.45       | 121.47   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 10  | C16   | 670  | GLU  | O-C-N      | -37.29 | 93.50       | 121.47   |
| 10  | C     | 670  | GLU  | O-C-N      | -37.29 | 93.50       | 121.47   |
| 10  | C32   | 670  | GLU  | O-C-N      | -37.22 | 93.55       | 121.47   |
| 10  | C16   | 1658 | ASP  | O-C-N      | -35.14 | 75.86       | 122.59   |
| 10  | C32   | 1658 | ASP  | O-C-N      | -35.12 | 75.88       | 122.59   |
| 10  | C24   | 1658 | ASP  | O-C-N      | -35.10 | 75.90       | 122.59   |
| 10  | C     | 1658 | ASP  | O-C-N      | -35.10 | 75.90       | 122.59   |
| 3   | N16   | 168  | VAL  | O-C-N      | -31.45 | 83.26       | 122.57   |
| 3   | N8    | 168  | VAL  | O-C-N      | -31.43 | 83.28       | 122.57   |
| 3   | N     | 168  | VAL  | O-C-N      | -31.40 | 83.32       | 122.57   |
| 1   | R16   | 1183 | GLU  | O-C-N      | -31.36 | 80.88       | 122.59   |
| 1   | R     | 1183 | GLU  | O-C-N      | -31.35 | 80.89       | 122.59   |
| 1   | R8    | 1183 | GLU  | O-C-N      | -31.33 | 80.92       | 122.59   |
| 9   | K8    | 1139 | ILE  | O-C-N      | -31.14 | 83.65       | 122.57   |
| 9   | K     | 1139 | ILE  | O-C-N      | -31.14 | 83.65       | 122.57   |
| 1   | R16   | 529  | HIS  | CG-CD2-NE2 | -29.67 | 77.53       | 107.20   |
| 1   | R     | 529  | HIS  | CG-CD2-NE2 | -29.66 | 77.53       | 107.20   |
| 1   | R8    | 529  | HIS  | CG-CD2-NE2 | -29.65 | 77.55       | 107.20   |
| 4   | T     | 160  | HIS  | CG-CD2-NE2 | -29.38 | 77.82       | 107.20   |
| 4   | T8    | 160  | HIS  | CG-CD2-NE2 | -29.38 | 77.83       | 107.20   |
| 4   | T16   | 160  | HIS  | CG-CD2-NE2 | -29.36 | 77.84       | 107.20   |
| 8   | L8    | 1054 | HIS  | CG-CD2-NE2 | -29.34 | 77.86       | 107.20   |
| 8   | L16   | 1054 | HIS  | CG-CD2-NE2 | -29.33 | 77.87       | 107.20   |
| 8   | L     | 1054 | HIS  | CG-CD2-NE2 | -29.32 | 77.88       | 107.20   |
| 18  | B     | 1476 | SER  | O-C-N      | -29.10 | 83.06       | 122.06   |
| 18  | B8    | 1476 | SER  | O-C-N      | -29.09 | 83.08       | 122.06   |
| 1   | R8    | 1189 | PRO  | O-C-N      | -27.23 | 85.88       | 122.64   |
| 1   | R16   | 1189 | PRO  | O-C-N      | -27.22 | 85.89       | 122.64   |
| 1   | R     | 1189 | PRO  | O-C-N      | -27.17 | 85.96       | 122.64   |
| 18  | B8    | 1116 | GLU  | O-C-N      | -26.62 | 87.19       | 122.59   |
| 18  | B     | 1116 | GLU  | O-C-N      | -26.58 | 87.24       | 122.59   |
| 9   | K8    | 1054 | THR  | O-C-N      | -26.44 | 87.42       | 122.59   |
| 9   | K     | 1054 | THR  | O-C-N      | -26.43 | 87.44       | 122.59   |
| 17  | F24   | 72   | SER  | O-C-N      | -26.40 | 87.47       | 122.59   |
| 17  | F16   | 72   | SER  | O-C-N      | -26.40 | 87.48       | 122.59   |
| 17  | F8    | 72   | SER  | O-C-N      | -26.39 | 87.49       | 122.59   |
| 17  | F     | 72   | SER  | O-C-N      | -26.39 | 87.49       | 122.59   |
| 9   | K     | 1051 | GLU  | O-C-N      | -26.30 | 87.62       | 122.59   |
| 9   | K8    | 1051 | GLU  | O-C-N      | -26.18 | 87.78       | 122.59   |
| 9   | K     | 1088 | ASP  | O-C-N      | -25.10 | 89.24       | 122.38   |
| 9   | K8    | 1088 | ASP  | O-C-N      | -25.09 | 89.26       | 122.38   |
| 10  | C     | 251  | GLY  | O-C-N      | -24.59 | 107.86      | 123.35   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 10  | C16   | 251  | GLY  | O-C-N       | -24.53 | 107.89      | 123.35   |
| 10  | C24   | 251  | GLY  | O-C-N       | -24.53 | 107.89      | 123.35   |
| 10  | C8    | 251  | GLY  | O-C-N       | -24.53 | 107.90      | 123.35   |
| 10  | C32   | 251  | GLY  | O-C-N       | -24.49 | 107.92      | 123.35   |
| 15  | J     | 677  | GLY  | O-C-N       | -24.29 | 91.12       | 122.70   |
| 19  | 4     | 445  | VAL  | O-C-N       | -24.21 | 92.30       | 122.57   |
| 19  | 48    | 445  | VAL  | O-C-N       | -24.15 | 92.38       | 122.57   |
| 10  | C24   | 1071 | GLN  | O-C-N       | -23.98 | 90.69       | 122.59   |
| 10  | C     | 1071 | GLN  | O-C-N       | -23.96 | 90.72       | 122.59   |
| 10  | C8    | 1071 | GLN  | O-C-N       | -23.95 | 90.73       | 122.59   |
| 10  | C32   | 1071 | GLN  | O-C-N       | -23.93 | 90.76       | 122.59   |
| 4   | T8    | 386  | HIS  | ND1-CE1-NE2 | -23.93 | 84.47       | 108.40   |
| 10  | C16   | 1071 | GLN  | O-C-N       | -23.92 | 90.78       | 122.59   |
| 4   | T16   | 386  | HIS  | ND1-CE1-NE2 | -23.91 | 84.49       | 108.40   |
| 9   | K     | 727  | ASP  | O-C-N       | -23.91 | 90.80       | 122.59   |
| 4   | T     | 386  | HIS  | ND1-CE1-NE2 | -23.89 | 84.50       | 108.40   |
| 9   | K8    | 727  | ASP  | O-C-N       | -23.89 | 90.82       | 122.59   |
| 9   | K     | 1056 | VAL  | O-C-N       | -23.79 | 92.83       | 122.57   |
| 9   | K8    | 1056 | VAL  | O-C-N       | -23.79 | 92.83       | 122.57   |
| 10  | C     | 1617 | ALA  | O-C-N       | -23.59 | 91.21       | 122.59   |
| 10  | C8    | 1617 | ALA  | O-C-N       | -23.56 | 91.25       | 122.59   |
| 10  | C24   | 1617 | ALA  | O-C-N       | -23.55 | 91.28       | 122.59   |
| 10  | C32   | 1617 | ALA  | O-C-N       | -23.54 | 91.28       | 122.59   |
| 20  | E8    | 339  | LYS  | O-C-N       | -23.50 | 91.33       | 122.59   |
| 10  | C16   | 1617 | ALA  | O-C-N       | -23.48 | 91.36       | 122.59   |
| 20  | E     | 339  | LYS  | O-C-N       | -23.48 | 91.37       | 122.59   |
| 18  | B     | 1130 | LEU  | O-C-N       | -23.35 | 91.54       | 122.59   |
| 18  | B8    | 1130 | LEU  | O-C-N       | -23.34 | 91.55       | 122.59   |
| 10  | C8    | 1272 | GLN  | O-C-N       | -23.13 | 85.18       | 122.42   |
| 10  | C16   | 1272 | GLN  | O-C-N       | -23.12 | 85.20       | 122.42   |
| 10  | C24   | 1272 | GLN  | O-C-N       | -23.10 | 85.23       | 122.42   |
| 10  | C     | 1272 | GLN  | O-C-N       | -23.07 | 85.27       | 122.42   |
| 10  | C32   | 1272 | GLN  | O-C-N       | -23.07 | 85.28       | 122.42   |
| 2   | M8    | 346  | VAL  | O-C-N       | -22.94 | 93.89       | 122.57   |
| 2   | M16   | 346  | VAL  | O-C-N       | -22.92 | 93.92       | 122.57   |
| 2   | M     | 346  | VAL  | O-C-N       | -22.87 | 93.98       | 122.57   |
| 20  | E8    | 350  | GLU  | O-C-N       | -22.68 | 92.42       | 122.59   |
| 20  | E     | 350  | GLU  | O-C-N       | -22.65 | 92.47       | 122.59   |
| 18  | B8    | 1800 | ARG  | O-C-N       | -22.58 | 92.56       | 122.59   |
| 18  | B     | 1800 | ARG  | O-C-N       | -22.56 | 92.58       | 122.59   |
| 13  | V     | 883  | PRO  | O-C-N       | -21.99 | 92.95       | 122.64   |
| 4   | T     | 386  | HIS  | CE1-NE2-CD2 | -21.97 | 87.03       | 109.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 4   | T16   | 386  | HIS  | CE1-NE2-CD2 | -21.96 | 87.04       | 109.00   |
| 4   | T8    | 386  | HIS  | CE1-NE2-CD2 | -21.92 | 87.08       | 109.00   |
| 4   | T16   | 386  | HIS  | CG-CD2-NE2  | 21.91  | 129.11      | 107.20   |
| 4   | T     | 386  | HIS  | CG-CD2-NE2  | 21.88  | 129.08      | 107.20   |
| 4   | T8    | 386  | HIS  | CG-CD2-NE2  | 21.86  | 129.06      | 107.20   |
| 19  | 4     | 60   | GLN  | O-C-N       | -21.60 | 93.86       | 122.59   |
| 19  | 48    | 60   | GLN  | O-C-N       | -21.60 | 93.87       | 122.59   |
| 18  | B     | 684  | ILE  | O-C-N       | -21.48 | 95.72       | 122.57   |
| 18  | B8    | 684  | ILE  | O-C-N       | -21.47 | 95.74       | 122.57   |
| 19  | 48    | 58   | GLU  | O-C-N       | -21.42 | 94.10       | 122.59   |
| 1   | R8    | 1197 | GLU  | O-C-N       | -21.37 | 88.02       | 122.42   |
| 19  | 4     | 58   | GLU  | O-C-N       | -21.37 | 94.17       | 122.59   |
| 1   | R16   | 1197 | GLU  | O-C-N       | -21.36 | 88.03       | 122.42   |
| 1   | R     | 1197 | GLU  | O-C-N       | -21.33 | 88.08       | 122.42   |
| 18  | B     | 970  | SER  | O-C-N       | -21.17 | 94.44       | 122.38   |
| 18  | B8    | 970  | SER  | O-C-N       | -21.16 | 94.45       | 122.38   |
| 19  | 48    | 56   | GLU  | O-C-N       | -21.12 | 94.50       | 122.59   |
| 19  | 4     | 56   | GLU  | O-C-N       | -21.08 | 94.55       | 122.59   |
| 9   | K8    | 722  | GLN  | O-C-N       | -20.83 | 100.37      | 122.03   |
| 18  | B     | 679  | ASP  | O-C-N       | -20.82 | 94.91       | 122.59   |
| 9   | K     | 722  | GLN  | O-C-N       | -20.77 | 100.43      | 122.03   |
| 10  | C16   | 1072 | ASP  | O-C-N       | -20.76 | 94.98       | 122.59   |
| 10  | C24   | 1072 | ASP  | O-C-N       | -20.76 | 94.98       | 122.59   |
| 10  | C     | 1072 | ASP  | O-C-N       | -20.75 | 94.99       | 122.59   |
| 10  | C32   | 1072 | ASP  | O-C-N       | -20.73 | 95.02       | 122.59   |
| 22  | I16   | 296  | ARG  | O-C-N       | -20.72 | 96.95       | 122.65   |
| 18  | B     | 1799 | VAL  | O-C-N       | -20.72 | 96.67       | 122.57   |
| 18  | B8    | 679  | ASP  | O-C-N       | -20.72 | 95.03       | 122.59   |
| 10  | C8    | 1056 | VAL  | O-C-N       | -20.71 | 96.68       | 122.57   |
| 10  | C     | 1056 | VAL  | O-C-N       | -20.71 | 96.68       | 122.57   |
| 18  | B8    | 1799 | VAL  | O-C-N       | -20.71 | 96.69       | 122.57   |
| 22  | I     | 296  | ARG  | O-C-N       | -20.71 | 96.97       | 122.65   |
| 22  | I8    | 296  | ARG  | O-C-N       | -20.71 | 96.97       | 122.65   |
| 22  | I24   | 296  | ARG  | O-C-N       | -20.69 | 96.99       | 122.65   |
| 19  | 4     | 71   | LYS  | CA-C-N      | 20.68  | 139.75      | 120.10   |
| 19  | 4     | 71   | LYS  | C-N-CA      | 20.68  | 139.75      | 120.10   |
| 10  | C16   | 1056 | VAL  | O-C-N       | -20.66 | 96.75       | 122.57   |
| 19  | 48    | 71   | LYS  | CA-C-N      | 20.66  | 139.73      | 120.10   |
| 19  | 48    | 71   | LYS  | C-N-CA      | 20.66  | 139.73      | 120.10   |
| 10  | C32   | 1056 | VAL  | O-C-N       | -20.66 | 96.75       | 122.57   |
| 10  | C8    | 1072 | ASP  | O-C-N       | -20.66 | 95.12       | 122.59   |
| 10  | C24   | 1056 | VAL  | O-C-N       | -20.65 | 96.76       | 122.57   |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10  | C     | 1620 | ILE  | O-C-N | -20.57 | 96.85       | 122.57   |
| 10  | C16   | 1620 | ILE  | O-C-N | -20.56 | 96.87       | 122.57   |
| 10  | C32   | 1620 | ILE  | O-C-N | -20.53 | 96.91       | 122.57   |
| 10  | C24   | 1620 | ILE  | O-C-N | -20.51 | 96.93       | 122.57   |
| 10  | C8    | 1620 | ILE  | O-C-N | -20.50 | 96.94       | 122.57   |
| 9   | K8    | 1274 | GLY  | O-C-N | -20.01 | 96.69       | 122.70   |
| 9   | K     | 1274 | GLY  | O-C-N | -19.99 | 96.71       | 122.70   |
| 10  | C24   | 1356 | ASP  | O-C-N | -19.99 | 96.01       | 122.59   |
| 10  | C     | 1356 | ASP  | O-C-N | -19.98 | 96.02       | 122.59   |
| 10  | C16   | 1356 | ASP  | O-C-N | -19.98 | 96.02       | 122.59   |
| 10  | C32   | 1356 | ASP  | O-C-N | -19.96 | 96.04       | 122.59   |
| 10  | C8    | 1356 | ASP  | O-C-N | -19.93 | 96.08       | 122.59   |
| 10  | C8    | 1128 | SER  | O-C-N | -19.90 | 96.13       | 122.59   |
| 10  | C16   | 1128 | SER  | O-C-N | -19.87 | 96.16       | 122.59   |
| 10  | C     | 1128 | SER  | O-C-N | -19.87 | 96.17       | 122.59   |
| 10  | C32   | 1128 | SER  | O-C-N | -19.85 | 96.19       | 122.59   |
| 9   | K     | 1277 | ALA  | O-C-N | -19.82 | 96.23       | 122.59   |
| 10  | C24   | 1128 | SER  | O-C-N | -19.80 | 96.26       | 122.59   |
| 9   | K8    | 1277 | ALA  | O-C-N | -19.75 | 96.32       | 122.59   |
| 13  | V     | 873  | GLY  | O-C-N | -19.55 | 97.28       | 122.70   |
| 18  | B     | 508  | ALA  | O-C-N | -19.47 | 95.03       | 122.29   |
| 18  | B8    | 508  | ALA  | O-C-N | -19.45 | 95.05       | 122.29   |
| 10  | C16   | 448  | LYS  | O-C-N | -19.41 | 96.78       | 122.59   |
| 9   | K8    | 929  | ARG  | O-C-N | -19.38 | 96.81       | 122.59   |
| 10  | C24   | 448  | LYS  | O-C-N | -19.37 | 96.83       | 122.59   |
| 18  | B     | 1113 | PRO  | O-C-N | -19.37 | 96.49       | 122.64   |
| 10  | C32   | 448  | LYS  | O-C-N | -19.36 | 96.84       | 122.59   |
| 7   | Q16   | 89   | GLY  | O-C-N | -19.35 | 97.54       | 122.70   |
| 18  | B8    | 1113 | PRO  | O-C-N | -19.33 | 96.55       | 122.64   |
| 18  | B8    | 674  | CYS  | O-C-N | -19.32 | 96.89       | 122.59   |
| 9   | K     | 929  | ARG  | O-C-N | -19.31 | 96.91       | 122.59   |
| 7   | Q8    | 89   | GLY  | O-C-N | -19.30 | 97.60       | 122.70   |
| 18  | B     | 674  | CYS  | O-C-N | -19.30 | 96.92       | 122.59   |
| 7   | Q     | 89   | GLY  | O-C-N | -19.26 | 97.66       | 122.70   |
| 18  | B     | 976  | SER  | O-C-N | -19.03 | 97.49       | 122.61   |
| 10  | C16   | 1619 | PRO  | O-C-N | -19.02 | 96.96       | 122.64   |
| 18  | B8    | 976  | SER  | O-C-N | -19.02 | 97.50       | 122.61   |
| 10  | C32   | 1619 | PRO  | O-C-N | -19.02 | 96.97       | 122.64   |
| 10  | C24   | 1619 | PRO  | O-C-N | -18.99 | 97.00       | 122.64   |
| 10  | C     | 1619 | PRO  | O-C-N | -18.98 | 97.02       | 122.64   |
| 5   | P16   | 392  | PRO  | O-C-N | -18.97 | 97.03       | 122.64   |
| 5   | P     | 392  | PRO  | O-C-N | -18.96 | 97.04       | 122.64   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 5   | P8    | 392  | PRO  | O-C-N  | -18.95 | 97.06       | 122.64   |
| 10  | C8    | 1619 | PRO  | O-C-N  | -18.93 | 97.08       | 122.64   |
| 20  | E8    | 435  | ALA  | O-C-N  | -18.90 | 97.45       | 122.59   |
| 20  | E     | 435  | ALA  | O-C-N  | -18.90 | 97.45       | 122.59   |
| 9   | K8    | 1049 | ASP  | O-C-N  | -18.88 | 100.12      | 122.22   |
| 1   | R     | 1205 | ASP  | O-C-N  | -18.88 | 97.48       | 122.59   |
| 1   | R8    | 1205 | ASP  | O-C-N  | -18.86 | 97.51       | 122.59   |
| 1   | R16   | 1205 | ASP  | O-C-N  | -18.82 | 97.56       | 122.59   |
| 9   | K     | 1049 | ASP  | O-C-N  | -18.75 | 100.28      | 122.22   |
| 13  | V     | 878  | ALA  | O-C-N  | -18.71 | 97.70       | 122.59   |
| 10  | C16   | 671  | LYS  | CA-C-N | 18.70  | 148.84      | 122.85   |
| 10  | C16   | 671  | LYS  | C-N-CA | 18.70  | 148.84      | 122.85   |
| 10  | C8    | 671  | LYS  | CA-C-N | 18.70  | 148.84      | 122.85   |
| 10  | C8    | 671  | LYS  | C-N-CA | 18.70  | 148.84      | 122.85   |
| 10  | C32   | 671  | LYS  | CA-C-N | 18.69  | 148.83      | 122.85   |
| 10  | C32   | 671  | LYS  | C-N-CA | 18.69  | 148.83      | 122.85   |
| 10  | C24   | 671  | LYS  | CA-C-N | 18.68  | 148.81      | 122.85   |
| 10  | C24   | 671  | LYS  | C-N-CA | 18.68  | 148.81      | 122.85   |
| 10  | C     | 671  | LYS  | CA-C-N | 18.68  | 148.81      | 122.85   |
| 10  | C     | 671  | LYS  | C-N-CA | 18.68  | 148.81      | 122.85   |
| 21  | H24   | 318  | ALA  | O-C-N  | -18.56 | 100.38      | 122.46   |
| 21  | H     | 318  | ALA  | O-C-N  | -18.55 | 100.38      | 122.46   |
| 21  | H8    | 318  | ALA  | O-C-N  | -18.55 | 100.39      | 122.46   |
| 21  | H16   | 318  | ALA  | O-C-N  | -18.55 | 100.39      | 122.46   |
| 11  | A24   | 159  | LYS  | O-C-N  | -18.50 | 97.99       | 122.59   |
| 11  | A40   | 159  | LYS  | O-C-N  | -18.48 | 98.02       | 122.59   |
| 12  | A48   | 159  | LYS  | O-C-N  | -18.46 | 98.04       | 122.59   |
| 12  | A     | 159  | LYS  | O-C-N  | -18.44 | 98.07       | 122.59   |
| 16  | A8    | 159  | LYS  | O-C-N  | -18.40 | 98.12       | 122.59   |
| 10  | C24   | 1063 | PRO  | O-C-N  | -18.34 | 97.89       | 122.64   |
| 10  | C32   | 1063 | PRO  | O-C-N  | -18.32 | 97.91       | 122.64   |
| 10  | C     | 1063 | PRO  | O-C-N  | -18.30 | 97.94       | 122.64   |
| 10  | C8    | 1063 | PRO  | O-C-N  | -18.27 | 97.98       | 122.64   |
| 10  | C8    | 1073 | GLY  | CA-C-N | 18.27  | 144.19      | 120.44   |
| 10  | C8    | 1073 | GLY  | C-N-CA | 18.27  | 144.19      | 120.44   |
| 10  | C16   | 1063 | PRO  | O-C-N  | -18.26 | 97.98       | 122.64   |
| 10  | C32   | 1073 | GLY  | CA-C-N | 18.23  | 144.14      | 120.44   |
| 10  | C32   | 1073 | GLY  | C-N-CA | 18.23  | 144.14      | 120.44   |
| 10  | C24   | 1073 | GLY  | CA-C-N | 18.23  | 144.14      | 120.44   |
| 10  | C24   | 1073 | GLY  | C-N-CA | 18.23  | 144.14      | 120.44   |
| 10  | C     | 1073 | GLY  | CA-C-N | 18.18  | 144.08      | 120.44   |
| 10  | C     | 1073 | GLY  | C-N-CA | 18.18  | 144.08      | 120.44   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C16   | 1073 | GLY  | CA-C-N | 18.17  | 144.06      | 120.44   |
| 10  | C16   | 1073 | GLY  | C-N-CA | 18.17  | 144.06      | 120.44   |
| 18  | B8    | 1229 | GLY  | O-C-N  | -18.01 | 99.28       | 122.70   |
| 10  | C     | 1080 | SER  | O-C-N  | -17.99 | 98.66       | 122.59   |
| 18  | B     | 1229 | GLY  | O-C-N  | -17.99 | 99.31       | 122.70   |
| 10  | C24   | 1080 | SER  | O-C-N  | -17.93 | 98.75       | 122.59   |
| 10  | C32   | 1080 | SER  | O-C-N  | -17.92 | 98.75       | 122.59   |
| 10  | C16   | 1080 | SER  | O-C-N  | -17.91 | 98.77       | 122.59   |
| 10  | C8    | 1080 | SER  | O-C-N  | -17.90 | 98.79       | 122.59   |
| 20  | E     | 431  | SER  | CA-C-N | 17.75  | 144.99      | 120.49   |
| 20  | E     | 431  | SER  | C-N-CA | 17.75  | 144.99      | 120.49   |
| 20  | E8    | 431  | SER  | CA-C-N | 17.74  | 144.97      | 120.49   |
| 20  | E8    | 431  | SER  | C-N-CA | 17.74  | 144.97      | 120.49   |
| 19  | 48    | 51   | PRO  | O-C-N  | -17.70 | 98.75       | 122.64   |
| 19  | 4     | 51   | PRO  | O-C-N  | -17.70 | 98.75       | 122.64   |
| 11  | A16   | 469  | VAL  | O-C-N  | -17.66 | 100.50      | 122.57   |
| 11  | A32   | 469  | VAL  | O-C-N  | -17.65 | 100.51      | 122.57   |
| 11  | A40   | 469  | VAL  | O-C-N  | -17.64 | 100.52      | 122.57   |
| 11  | A24   | 469  | VAL  | O-C-N  | -17.62 | 100.55      | 122.57   |
| 12  | A48   | 469  | VAL  | O-C-N  | -17.59 | 100.58      | 122.57   |
| 12  | A     | 469  | VAL  | O-C-N  | -17.57 | 100.61      | 122.57   |
| 14  | W     | 702  | PRO  | O-C-N  | -17.44 | 99.09       | 122.64   |
| 9   | K     | 1053 | MET  | O-C-N  | -17.42 | 103.65      | 122.12   |
| 9   | K8    | 1053 | MET  | O-C-N  | -17.41 | 103.67      | 122.12   |
| 1   | R     | 1208 | LYS  | O-C-N  | -17.25 | 99.64       | 122.59   |
| 1   | R8    | 1208 | LYS  | O-C-N  | -17.24 | 99.66       | 122.59   |
| 1   | R16   | 1208 | LYS  | O-C-N  | -17.22 | 99.69       | 122.59   |
| 2   | M16   | 156  | GLY  | O-C-N  | -17.20 | 95.48       | 123.00   |
| 2   | M8    | 156  | GLY  | O-C-N  | -17.15 | 95.56       | 123.00   |
| 2   | M     | 156  | GLY  | O-C-N  | -17.09 | 95.66       | 123.00   |
| 19  | 48    | 186  | GLY  | O-C-N  | -17.07 | 100.51      | 122.70   |
| 19  | 4     | 186  | GLY  | O-C-N  | -17.04 | 100.55      | 122.70   |
| 18  | B8    | 854  | SER  | O-C-N  | -16.96 | 101.61      | 122.65   |
| 14  | W     | 585  | ILE  | O-C-N  | -16.93 | 101.41      | 122.57   |
| 18  | B     | 854  | SER  | O-C-N  | -16.90 | 101.70      | 122.65   |
| 9   | K     | 1234 | ARG  | O-C-N  | -16.73 | 100.34      | 122.59   |
| 9   | K8    | 1234 | ARG  | O-C-N  | -16.73 | 100.34      | 122.59   |
| 14  | W     | 704  | THR  | O-C-N  | -16.72 | 100.35      | 122.59   |
| 5   | P16   | 145  | ILE  | O-C-N  | -16.66 | 101.75      | 122.57   |
| 5   | P8    | 145  | ILE  | O-C-N  | -16.64 | 101.76      | 122.57   |
| 5   | P     | 145  | ILE  | O-C-N  | -16.61 | 101.80      | 122.57   |
| 10  | C8    | 1082 | ILE  | O-C-N  | -16.61 | 101.80      | 122.57   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 18  | B     | 1064 | ILE  | O-C-N  | -16.59 | 101.83      | 122.57   |
| 10  | C     | 669  | GLY  | O-C-N  | -16.58 | 101.14      | 122.70   |
| 10  | C24   | 1082 | ILE  | O-C-N  | -16.57 | 101.85      | 122.57   |
| 18  | B8    | 1064 | ILE  | O-C-N  | -16.57 | 101.86      | 122.57   |
| 10  | C32   | 1082 | ILE  | O-C-N  | -16.55 | 101.88      | 122.57   |
| 10  | C32   | 669  | GLY  | O-C-N  | -16.55 | 101.19      | 122.70   |
| 10  | C24   | 669  | GLY  | O-C-N  | -16.54 | 101.19      | 122.70   |
| 10  | C     | 1082 | ILE  | O-C-N  | -16.53 | 101.90      | 122.57   |
| 10  | C8    | 669  | GLY  | O-C-N  | -16.53 | 101.22      | 122.70   |
| 10  | C16   | 1082 | ILE  | O-C-N  | -16.51 | 101.93      | 122.57   |
| 20  | E8    | 429  | PRO  | O-C-N  | -16.51 | 100.35      | 122.64   |
| 10  | C16   | 669  | GLY  | O-C-N  | -16.49 | 101.26      | 122.70   |
| 18  | B8    | 1480 | HIS  | CA-C-N | 16.48  | 142.78      | 120.54   |
| 18  | B8    | 1480 | HIS  | C-N-CA | 16.48  | 142.78      | 120.54   |
| 20  | E     | 429  | PRO  | O-C-N  | -16.47 | 100.41      | 122.64   |
| 18  | B     | 1480 | HIS  | CA-C-N | 16.45  | 142.74      | 120.54   |
| 18  | B     | 1480 | HIS  | C-N-CA | 16.45  | 142.74      | 120.54   |
| 10  | C8    | 280  | SER  | O-C-N  | -16.41 | 98.02       | 122.96   |
| 10  | C32   | 280  | SER  | O-C-N  | -16.36 | 98.09       | 122.96   |
| 10  | C     | 280  | SER  | O-C-N  | -16.33 | 98.14       | 122.96   |
| 10  | C16   | 280  | SER  | O-C-N  | -16.32 | 98.15       | 122.96   |
| 10  | C24   | 280  | SER  | O-C-N  | -16.32 | 98.15       | 122.96   |
| 2   | M8    | 340  | GLU  | O-C-N  | -16.27 | 100.95      | 122.59   |
| 2   | M     | 340  | GLU  | O-C-N  | -16.26 | 100.96      | 122.59   |
| 9   | K8    | 1278 | GLU  | O-C-N  | -16.20 | 101.04      | 122.59   |
| 2   | M16   | 340  | GLU  | O-C-N  | -16.19 | 101.06      | 122.59   |
| 9   | K     | 1278 | GLU  | O-C-N  | -16.16 | 101.10      | 122.59   |
| 18  | B8    | 673  | SER  | O-C-N  | -16.15 | 101.11      | 122.59   |
| 18  | B     | 1066 | ASP  | O-C-N  | -16.13 | 101.13      | 122.59   |
| 18  | B8    | 1066 | ASP  | O-C-N  | -16.11 | 101.17      | 122.59   |
| 18  | B     | 673  | SER  | O-C-N  | -16.10 | 101.17      | 122.59   |
| 18  | B8    | 990  | PRO  | O-C-N  | -16.01 | 101.03      | 122.64   |
| 20  | E8    | 441  | ARG  | O-C-N  | -15.99 | 101.32      | 122.59   |
| 20  | E     | 441  | ARG  | O-C-N  | -15.98 | 101.34      | 122.59   |
| 12  | A     | 782  | PRO  | O-C-N  | -15.93 | 105.26      | 123.10   |
| 19  | 48    | 100  | ILE  | O-C-N  | -15.92 | 102.67      | 122.57   |
| 12  | A48   | 782  | PRO  | O-C-N  | -15.92 | 105.27      | 123.10   |
| 19  | 4     | 100  | ILE  | O-C-N  | -15.92 | 102.67      | 122.57   |
| 18  | B     | 990  | PRO  | O-C-N  | -15.90 | 101.17      | 122.64   |
| 10  | C32   | 1270 | SER  | O-C-N  | -15.90 | 103.23      | 122.63   |
| 10  | C     | 1270 | SER  | O-C-N  | -15.89 | 103.25      | 122.63   |
| 18  | B8    | 689  | SER  | O-C-N  | -15.88 | 101.47      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C16   | 1270 | SER  | O-C-N  | -15.87 | 103.27      | 122.63   |
| 10  | C24   | 1270 | SER  | O-C-N  | -15.85 | 103.30      | 122.63   |
| 11  | A16   | 782  | PRO  | O-C-N  | -15.83 | 105.37      | 123.10   |
| 10  | C8    | 1270 | SER  | O-C-N  | -15.83 | 103.32      | 122.63   |
| 18  | B     | 689  | SER  | O-C-N  | -15.83 | 101.54      | 122.59   |
| 11  | A24   | 782  | PRO  | O-C-N  | -15.83 | 105.38      | 123.10   |
| 11  | A40   | 782  | PRO  | O-C-N  | -15.83 | 105.37      | 123.10   |
| 11  | A32   | 782  | PRO  | O-C-N  | -15.81 | 105.39      | 123.10   |
| 13  | V     | 879  | ARG  | O-C-N  | -15.70 | 101.71      | 122.59   |
| 17  | F     | 70   | PRO  | O-C-N  | -15.57 | 101.62      | 122.64   |
| 17  | F24   | 70   | PRO  | O-C-N  | -15.53 | 101.68      | 122.64   |
| 17  | F8    | 70   | PRO  | O-C-N  | -15.51 | 101.71      | 122.64   |
| 10  | C8    | 1287 | MET  | O-C-N  | -15.49 | 103.34      | 122.71   |
| 10  | C24   | 1778 | ASN  | O-C-N  | -15.49 | 105.92      | 122.03   |
| 10  | C24   | 1053 | GLY  | O-C-N  | -15.48 | 102.58      | 122.70   |
| 17  | F16   | 70   | PRO  | O-C-N  | -15.48 | 101.74      | 122.64   |
| 10  | C24   | 1287 | MET  | O-C-N  | -15.47 | 103.38      | 122.71   |
| 10  | C32   | 1287 | MET  | O-C-N  | -15.47 | 103.37      | 122.71   |
| 10  | C32   | 1778 | ASN  | O-C-N  | -15.45 | 105.97      | 122.03   |
| 10  | C16   | 1287 | MET  | O-C-N  | -15.44 | 103.41      | 122.71   |
| 10  | C     | 1287 | MET  | O-C-N  | -15.44 | 103.42      | 122.71   |
| 10  | C16   | 1778 | ASN  | O-C-N  | -15.43 | 105.98      | 122.03   |
| 10  | C8    | 1053 | GLY  | O-C-N  | -15.41 | 102.67      | 122.70   |
| 10  | C8    | 1778 | ASN  | O-C-N  | -15.39 | 106.03      | 122.03   |
| 10  | C     | 1053 | GLY  | O-C-N  | -15.38 | 102.70      | 122.70   |
| 10  | C32   | 1053 | GLY  | O-C-N  | -15.37 | 102.72      | 122.70   |
| 18  | B     | 1111 | LYS  | O-C-N  | -15.35 | 102.12      | 122.38   |
| 10  | C     | 1778 | ASN  | O-C-N  | -15.34 | 106.08      | 122.03   |
| 18  | B8    | 1111 | LYS  | O-C-N  | -15.33 | 102.15      | 122.38   |
| 10  | C16   | 1053 | GLY  | O-C-N  | -15.32 | 102.78      | 122.70   |
| 10  | C32   | 667  | ILE  | CA-C-N | -15.32 | 92.28       | 121.54   |
| 10  | C32   | 667  | ILE  | C-N-CA | -15.32 | 92.28       | 121.54   |
| 10  | C16   | 667  | ILE  | CA-C-N | -15.32 | 92.28       | 121.54   |
| 10  | C16   | 667  | ILE  | C-N-CA | -15.32 | 92.28       | 121.54   |
| 19  | 4     | 91   | PRO  | O-C-N  | -15.31 | 101.97      | 122.64   |
| 19  | 48    | 91   | PRO  | O-C-N  | -15.31 | 101.97      | 122.64   |
| 10  | C24   | 667  | ILE  | CA-C-N | -15.30 | 92.31       | 121.54   |
| 10  | C24   | 667  | ILE  | C-N-CA | -15.30 | 92.31       | 121.54   |
| 10  | C8    | 667  | ILE  | CA-C-N | -15.30 | 92.32       | 121.54   |
| 10  | C8    | 667  | ILE  | C-N-CA | -15.30 | 92.32       | 121.54   |
| 10  | C     | 667  | ILE  | CA-C-N | -15.29 | 92.34       | 121.54   |
| 10  | C     | 667  | ILE  | C-N-CA | -15.29 | 92.34       | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 7   | Q8    | 90   | GLY  | CA-C-N | 15.15  | 151.11      | 121.41   |
| 7   | Q8    | 90   | GLY  | C-N-CA | 15.15  | 151.11      | 121.41   |
| 7   | Q16   | 90   | GLY  | CA-C-N | 15.15  | 151.10      | 121.41   |
| 7   | Q16   | 90   | GLY  | C-N-CA | 15.15  | 151.10      | 121.41   |
| 7   | Q     | 90   | GLY  | CA-C-N | 15.14  | 151.09      | 121.41   |
| 7   | Q     | 90   | GLY  | C-N-CA | 15.14  | 151.09      | 121.41   |
| 9   | K     | 1090 | ASP  | CA-C-N | 14.99  | 141.63      | 120.79   |
| 9   | K     | 1090 | ASP  | C-N-CA | 14.99  | 141.63      | 120.79   |
| 18  | B8    | 907  | SER  | O-C-N  | -14.97 | 104.64      | 122.46   |
| 9   | K8    | 1090 | ASP  | CA-C-N | 14.97  | 141.60      | 120.79   |
| 9   | K8    | 1090 | ASP  | C-N-CA | 14.97  | 141.60      | 120.79   |
| 18  | B     | 907  | SER  | O-C-N  | -14.94 | 104.68      | 122.46   |
| 9   | K     | 1065 | GLU  | O-C-N  | -14.93 | 102.74      | 122.59   |
| 9   | K8    | 1065 | GLU  | O-C-N  | -14.93 | 102.74      | 122.59   |
| 18  | B8    | 1479 | GLY  | O-C-N  | -14.87 | 103.37      | 122.70   |
| 18  | B     | 1479 | GLY  | O-C-N  | -14.84 | 103.41      | 122.70   |
| 22  | I24   | 252  | ARG  | O-C-N  | -14.84 | 99.27       | 123.00   |
| 18  | B     | 1742 | SER  | O-C-N  | -14.83 | 102.22      | 122.68   |
| 22  | I     | 252  | ARG  | O-C-N  | -14.83 | 99.28       | 123.00   |
| 15  | J     | 682  | ALA  | O-C-N  | -14.82 | 103.05      | 122.61   |
| 22  | I8    | 252  | ARG  | O-C-N  | -14.82 | 99.29       | 123.00   |
| 22  | I16   | 252  | ARG  | O-C-N  | -14.82 | 99.29       | 123.00   |
| 18  | B8    | 1742 | SER  | O-C-N  | -14.80 | 102.25      | 122.68   |
| 17  | F16   | 77   | TYR  | O-C-N  | -14.72 | 105.54      | 123.05   |
| 5   | P16   | 13   | LEU  | O-C-N  | -14.71 | 103.03      | 122.59   |
| 17  | F8    | 77   | TYR  | O-C-N  | -14.71 | 105.55      | 123.05   |
| 10  | C24   | 1543 | GLU  | O-C-N  | -14.70 | 103.04      | 122.59   |
| 5   | P8    | 13   | LEU  | O-C-N  | -14.69 | 103.05      | 122.59   |
| 5   | P     | 13   | LEU  | O-C-N  | -14.68 | 103.07      | 122.59   |
| 2   | M     | 350  | SER  | O-C-N  | -14.66 | 103.09      | 122.59   |
| 17  | F24   | 77   | TYR  | O-C-N  | -14.66 | 105.60      | 123.05   |
| 17  | F     | 77   | TYR  | O-C-N  | -14.66 | 105.60      | 123.05   |
| 10  | C16   | 1543 | GLU  | O-C-N  | -14.66 | 103.09      | 122.59   |
| 10  | C32   | 1543 | GLU  | O-C-N  | -14.65 | 103.10      | 122.59   |
| 2   | M16   | 350  | SER  | O-C-N  | -14.65 | 103.11      | 122.59   |
| 2   | M8    | 350  | SER  | O-C-N  | -14.64 | 103.12      | 122.59   |
| 10  | C16   | 1081 | SER  | O-C-N  | -14.63 | 103.14      | 122.59   |
| 10  | C32   | 1081 | SER  | O-C-N  | -14.62 | 103.14      | 122.59   |
| 22  | I24   | 209  | TRP  | O-C-N  | -14.62 | 101.82      | 122.29   |
| 10  | C8    | 1543 | GLU  | O-C-N  | -14.61 | 103.16      | 122.59   |
| 10  | C24   | 1081 | SER  | O-C-N  | -14.60 | 103.17      | 122.59   |
| 22  | I16   | 209  | TRP  | O-C-N  | -14.57 | 101.89      | 122.29   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 22  | I     | 209  | TRP  | O-C-N  | -14.57 | 101.89      | 122.29   |
| 10  | C     | 1081 | SER  | O-C-N  | -14.57 | 103.22      | 122.59   |
| 10  | C8    | 1081 | SER  | O-C-N  | -14.56 | 103.23      | 122.59   |
| 7   | Q     | 92   | GLY  | O-C-N  | -14.55 | 103.78      | 122.70   |
| 22  | I8    | 209  | TRP  | O-C-N  | -14.54 | 101.94      | 122.29   |
| 10  | C24   | 1662 | ASP  | CA-C-N | 14.52  | 141.27      | 120.95   |
| 10  | C24   | 1662 | ASP  | C-N-CA | 14.52  | 141.27      | 120.95   |
| 10  | C     | 1662 | ASP  | CA-C-N | 14.51  | 141.27      | 120.95   |
| 10  | C     | 1662 | ASP  | C-N-CA | 14.51  | 141.27      | 120.95   |
| 7   | Q8    | 92   | GLY  | O-C-N  | -14.50 | 103.85      | 122.70   |
| 18  | B     | 1786 | PRO  | O-C-N  | -14.49 | 103.08      | 122.64   |
| 10  | C16   | 1662 | ASP  | CA-C-N | 14.49  | 141.23      | 120.95   |
| 10  | C16   | 1662 | ASP  | C-N-CA | 14.49  | 141.23      | 120.95   |
| 18  | B8    | 981  | GLN  | O-C-N  | -14.49 | 103.32      | 122.59   |
| 10  | C     | 1495 | SER  | O-C-N  | -14.48 | 103.59      | 122.56   |
| 10  | C32   | 1662 | ASP  | CA-C-N | 14.48  | 141.22      | 120.95   |
| 10  | C32   | 1662 | ASP  | C-N-CA | 14.48  | 141.22      | 120.95   |
| 18  | B     | 981  | GLN  | O-C-N  | -14.47 | 103.34      | 122.59   |
| 10  | C32   | 1495 | SER  | O-C-N  | -14.47 | 103.61      | 122.56   |
| 18  | B8    | 1786 | PRO  | O-C-N  | -14.46 | 103.11      | 122.64   |
| 10  | C24   | 1495 | SER  | O-C-N  | -14.46 | 103.62      | 122.56   |
| 10  | C8    | 1495 | SER  | O-C-N  | -14.45 | 103.63      | 122.56   |
| 18  | B8    | 192  | PRO  | O-C-N  | -14.43 | 103.16      | 122.64   |
| 10  | C16   | 1495 | SER  | O-C-N  | -14.42 | 103.67      | 122.56   |
| 7   | Q16   | 92   | GLY  | O-C-N  | -14.41 | 103.96      | 122.70   |
| 18  | B     | 192  | PRO  | O-C-N  | -14.40 | 103.19      | 122.64   |
| 18  | B8    | 992  | TRP  | O-C-N  | -14.39 | 103.45      | 122.59   |
| 18  | B     | 992  | TRP  | O-C-N  | -14.38 | 103.46      | 122.59   |
| 10  | C16   | 1662 | ASP  | O-C-N  | -14.34 | 103.52      | 122.59   |
| 9   | K     | 1047 | SER  | O-C-N  | -14.31 | 103.55      | 122.59   |
| 10  | C24   | 1662 | ASP  | O-C-N  | -14.30 | 103.57      | 122.59   |
| 10  | C32   | 1662 | ASP  | O-C-N  | -14.30 | 103.58      | 122.59   |
| 1   | R8    | 1185 | THR  | O-C-N  | -14.29 | 103.59      | 122.59   |
| 1   | R16   | 1185 | THR  | O-C-N  | -14.26 | 103.63      | 122.59   |
| 1   | R     | 1185 | THR  | O-C-N  | -14.25 | 103.63      | 122.59   |
| 9   | K8    | 1047 | SER  | O-C-N  | -14.25 | 103.64      | 122.59   |
| 10  | C     | 1662 | ASP  | O-C-N  | -14.25 | 103.64      | 122.59   |
| 10  | C     | 624  | GLY  | O-C-N  | -14.22 | 104.22      | 122.70   |
| 10  | C8    | 672  | ASP  | O-C-N  | -14.19 | 105.42      | 122.87   |
| 10  | C32   | 447  | PHE  | O-C-N  | -14.19 | 103.72      | 122.59   |
| 10  | C24   | 672  | ASP  | O-C-N  | -14.17 | 105.44      | 122.87   |
| 10  | C32   | 624  | GLY  | O-C-N  | -14.17 | 104.28      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C32   | 672  | ASP  | O-C-N  | -14.16 | 105.45      | 122.87   |
| 10  | C16   | 672  | ASP  | O-C-N  | -14.16 | 105.46      | 122.87   |
| 13  | V     | 820  | ASP  | CA-C-N | 14.15  | 139.77      | 120.38   |
| 13  | V     | 820  | ASP  | C-N-CA | 14.15  | 139.77      | 120.38   |
| 10  | C     | 672  | ASP  | O-C-N  | -14.15 | 105.47      | 122.87   |
| 10  | C24   | 624  | GLY  | O-C-N  | -14.13 | 104.33      | 122.70   |
| 18  | B     | 612  | GLY  | O-C-N  | -14.13 | 110.33      | 122.77   |
| 10  | C16   | 447  | PHE  | O-C-N  | -14.12 | 103.80      | 122.59   |
| 10  | C16   | 624  | GLY  | O-C-N  | -14.12 | 104.35      | 122.70   |
| 18  | B8    | 612  | GLY  | O-C-N  | -14.11 | 110.36      | 122.77   |
| 10  | C24   | 447  | PHE  | O-C-N  | -14.09 | 103.85      | 122.59   |
| 2   | M8    | 349  | ASP  | O-C-N  | -14.05 | 103.91      | 122.59   |
| 9   | K8    | 1060 | THR  | O-C-N  | -14.04 | 105.96      | 122.11   |
| 20  | E     | 207  | LEU  | O-C-N  | -14.04 | 103.92      | 122.59   |
| 20  | E8    | 207  | LEU  | O-C-N  | -14.04 | 103.92      | 122.59   |
| 19  | 48    | 63   | GLY  | CA-C-N | -14.01 | 94.77       | 121.54   |
| 19  | 48    | 63   | GLY  | C-N-CA | -14.01 | 94.77       | 121.54   |
| 9   | K     | 1060 | THR  | O-C-N  | -13.99 | 106.02      | 122.11   |
| 19  | 4     | 63   | GLY  | CA-C-N | -13.99 | 94.82       | 121.54   |
| 19  | 4     | 63   | GLY  | C-N-CA | -13.99 | 94.82       | 121.54   |
| 2   | M16   | 349  | ASP  | O-C-N  | -13.99 | 103.99      | 122.59   |
| 20  | E     | 203  | TRP  | O-C-N  | -13.98 | 103.99      | 122.59   |
| 2   | M     | 349  | ASP  | O-C-N  | -13.97 | 104.01      | 122.59   |
| 20  | E8    | 203  | TRP  | O-C-N  | -13.96 | 104.02      | 122.59   |
| 20  | E8    | 432  | ILE  | CA-C-N | 13.94  | 148.16      | 121.54   |
| 20  | E8    | 432  | ILE  | C-N-CA | 13.94  | 148.16      | 121.54   |
| 10  | C32   | 1623 | ILE  | O-C-N  | -13.93 | 105.15      | 122.57   |
| 20  | E     | 432  | ILE  | CA-C-N | 13.91  | 148.11      | 121.54   |
| 20  | E     | 432  | ILE  | C-N-CA | 13.91  | 148.11      | 121.54   |
| 10  | C16   | 1623 | ILE  | O-C-N  | -13.90 | 105.19      | 122.57   |
| 10  | C     | 1623 | ILE  | O-C-N  | -13.86 | 105.25      | 122.57   |
| 2   | M     | 527  | GLY  | CA-C-N | 13.85  | 141.19      | 121.24   |
| 2   | M     | 527  | GLY  | C-N-CA | 13.85  | 141.19      | 121.24   |
| 10  | C24   | 1623 | ILE  | O-C-N  | -13.85 | 105.25      | 122.57   |
| 10  | C8    | 1623 | ILE  | O-C-N  | -13.85 | 105.25      | 122.57   |
| 2   | M16   | 527  | GLY  | CA-C-N | 13.80  | 141.11      | 121.24   |
| 2   | M16   | 527  | GLY  | C-N-CA | 13.80  | 141.11      | 121.24   |
| 2   | M8    | 527  | GLY  | CA-C-N | 13.79  | 141.10      | 121.24   |
| 2   | M8    | 527  | GLY  | C-N-CA | 13.79  | 141.10      | 121.24   |
| 1   | R16   | 1188 | TYR  | O-C-N  | -13.79 | 110.71      | 121.47   |
| 21  | H8    | 319  | GLY  | O-C-N  | -13.72 | 104.87      | 122.70   |
| 1   | R     | 1188 | TYR  | O-C-N  | -13.71 | 110.78      | 121.47   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C     | 716  | THR  | CA-C-N | 13.70  | 141.13      | 120.31   |
| 10  | C     | 716  | THR  | C-N-CA | 13.70  | 141.13      | 120.31   |
| 10  | C24   | 716  | THR  | CA-C-N | 13.69  | 141.11      | 120.31   |
| 10  | C24   | 716  | THR  | C-N-CA | 13.69  | 141.11      | 120.31   |
| 18  | B8    | 1117 | THR  | CA-C-N | 13.69  | 140.94      | 120.82   |
| 18  | B8    | 1117 | THR  | C-N-CA | 13.69  | 140.94      | 120.82   |
| 1   | R8    | 1188 | TYR  | O-C-N  | -13.68 | 110.80      | 121.47   |
| 10  | C32   | 716  | THR  | CA-C-N | 13.68  | 141.10      | 120.31   |
| 10  | C32   | 716  | THR  | C-N-CA | 13.68  | 141.10      | 120.31   |
| 10  | C16   | 716  | THR  | CA-C-N | 13.68  | 141.10      | 120.31   |
| 10  | C16   | 716  | THR  | C-N-CA | 13.68  | 141.10      | 120.31   |
| 21  | H     | 319  | GLY  | O-C-N  | -13.68 | 104.92      | 122.70   |
| 21  | H24   | 319  | GLY  | O-C-N  | -13.67 | 104.94      | 122.70   |
| 18  | B     | 1117 | THR  | CA-C-N | 13.66  | 140.91      | 120.82   |
| 18  | B     | 1117 | THR  | C-N-CA | 13.66  | 140.91      | 120.82   |
| 21  | H16   | 319  | GLY  | O-C-N  | -13.65 | 104.95      | 122.70   |
| 18  | B8    | 1287 | LEU  | O-C-N  | -13.64 | 104.96      | 122.83   |
| 10  | C24   | 1443 | ASP  | O-C-N  | -13.62 | 104.72      | 122.56   |
| 12  | A     | 465  | SER  | O-C-N  | -13.62 | 104.48      | 122.59   |
| 18  | B     | 1675 | LYS  | O-C-N  | -13.62 | 104.48      | 122.59   |
| 18  | B8    | 1675 | LYS  | O-C-N  | -13.61 | 104.48      | 122.59   |
| 10  | C16   | 1443 | ASP  | O-C-N  | -13.61 | 104.73      | 122.56   |
| 10  | C32   | 1443 | ASP  | O-C-N  | -13.60 | 104.74      | 122.56   |
| 12  | A48   | 465  | SER  | O-C-N  | -13.60 | 104.50      | 122.59   |
| 11  | A24   | 465  | SER  | O-C-N  | -13.59 | 104.51      | 122.59   |
| 10  | C     | 1443 | ASP  | O-C-N  | -13.59 | 104.76      | 122.56   |
| 11  | A40   | 465  | SER  | O-C-N  | -13.58 | 104.53      | 122.59   |
| 5   | P16   | 11   | GLY  | O-C-N  | -13.58 | 105.05      | 122.70   |
| 18  | B     | 1287 | LEU  | O-C-N  | -13.58 | 105.04      | 122.83   |
| 18  | B8    | 613  | LYS  | O-C-N  | -13.58 | 104.53      | 122.59   |
| 11  | A16   | 465  | SER  | O-C-N  | -13.57 | 104.54      | 122.59   |
| 5   | P     | 11   | GLY  | O-C-N  | -13.56 | 105.08      | 122.70   |
| 18  | B     | 613  | LYS  | O-C-N  | -13.55 | 104.56      | 122.59   |
| 5   | P8    | 11   | GLY  | O-C-N  | -13.54 | 105.10      | 122.70   |
| 11  | A32   | 465  | SER  | O-C-N  | -13.54 | 104.58      | 122.59   |
| 18  | B8    | 1605 | GLU  | CA-C-N | 13.52  | 139.02      | 120.63   |
| 18  | B8    | 1605 | GLU  | C-N-CA | 13.52  | 139.02      | 120.63   |
| 18  | B8    | 1125 | VAL  | O-C-N  | -13.51 | 105.69      | 122.57   |
| 9   | K     | 1063 | GLU  | O-C-N  | -13.47 | 105.83      | 121.32   |
| 10  | C8    | 1443 | ASP  | O-C-N  | -13.47 | 104.92      | 122.56   |
| 18  | B     | 1125 | VAL  | O-C-N  | -13.46 | 105.74      | 122.57   |
| 18  | B     | 1605 | GLU  | CA-C-N | 13.45  | 138.93      | 120.63   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 18  | B     | 1605 | GLU  | C-N-CA | 13.45  | 138.93      | 120.63   |
| 10  | C32   | 1358 | ASP  | O-C-N  | -13.44 | 104.72      | 122.59   |
| 9   | K8    | 1063 | GLU  | O-C-N  | -13.43 | 105.87      | 121.32   |
| 14  | W     | 766  | LYS  | O-C-N  | -13.42 | 104.74      | 122.59   |
| 10  | C24   | 1065 | SER  | O-C-N  | -13.40 | 104.77      | 122.59   |
| 10  | C16   | 1358 | ASP  | O-C-N  | -13.40 | 104.77      | 122.59   |
| 13  | V     | 886  | SER  | O-C-N  | -13.39 | 104.93      | 122.61   |
| 10  | C8    | 1065 | SER  | O-C-N  | -13.39 | 104.78      | 122.59   |
| 10  | C16   | 1065 | SER  | O-C-N  | -13.39 | 104.78      | 122.59   |
| 10  | C     | 1065 | SER  | O-C-N  | -13.38 | 104.79      | 122.59   |
| 18  | B8    | 1680 | SER  | O-C-N  | -13.38 | 104.79      | 122.59   |
| 18  | B     | 610  | VAL  | O-C-N  | -13.38 | 105.85      | 122.57   |
| 18  | B     | 1680 | SER  | O-C-N  | -13.37 | 104.80      | 122.59   |
| 10  | C32   | 1065 | SER  | O-C-N  | -13.37 | 104.81      | 122.59   |
| 18  | B8    | 610  | VAL  | O-C-N  | -13.36 | 105.87      | 122.57   |
| 10  | C24   | 1358 | ASP  | O-C-N  | -13.34 | 104.85      | 122.59   |
| 9   | K     | 1273 | GLU  | O-C-N  | -13.33 | 104.86      | 122.59   |
| 10  | C8    | 1358 | ASP  | O-C-N  | -13.33 | 104.86      | 122.59   |
| 10  | C     | 1358 | ASP  | O-C-N  | -13.31 | 104.89      | 122.59   |
| 15  | J     | 679  | GLU  | O-C-N  | -13.31 | 104.89      | 122.59   |
| 9   | K8    | 1273 | GLU  | O-C-N  | -13.28 | 104.92      | 122.59   |
| 10  | C     | 633  | SER  | O-C-N  | -13.26 | 104.95      | 122.59   |
| 10  | C32   | 633  | SER  | O-C-N  | -13.21 | 105.02      | 122.59   |
| 18  | B8    | 1227 | TYR  | O-C-N  | -13.19 | 104.55      | 122.48   |
| 10  | C16   | 633  | SER  | O-C-N  | -13.18 | 105.06      | 122.59   |
| 10  | C24   | 633  | SER  | O-C-N  | -13.18 | 105.06      | 122.59   |
| 18  | B     | 1809 | SER  | O-C-N  | -13.18 | 106.78      | 122.46   |
| 18  | B8    | 1809 | SER  | O-C-N  | -13.15 | 106.81      | 122.46   |
| 2   | M8    | 761  | PRO  | O-C-N  | -13.15 | 104.89      | 122.64   |
| 2   | M     | 761  | PRO  | O-C-N  | -13.15 | 104.89      | 122.64   |
| 18  | B8    | 1605 | GLU  | O-C-N  | -13.15 | 105.11      | 122.59   |
| 1   | R     | 1193 | ALA  | O-C-N  | -13.14 | 105.34      | 122.56   |
| 14  | W     | 587  | SER  | CA-C-N | 13.13  | 142.65      | 120.72   |
| 14  | W     | 587  | SER  | C-N-CA | 13.13  | 142.65      | 120.72   |
| 1   | R16   | 1193 | ALA  | O-C-N  | -13.11 | 105.39      | 122.56   |
| 2   | M16   | 761  | PRO  | O-C-N  | -13.11 | 104.94      | 122.64   |
| 10  | C     | 623  | VAL  | O-C-N  | -13.09 | 106.21      | 122.57   |
| 1   | R8    | 1193 | ALA  | O-C-N  | -13.08 | 105.42      | 122.56   |
| 18  | B     | 1605 | GLU  | O-C-N  | -13.07 | 105.21      | 122.59   |
| 18  | B     | 1227 | TYR  | O-C-N  | -13.06 | 104.72      | 122.48   |
| 18  | B8    | 984  | LYS  | O-C-N  | -13.04 | 105.24      | 122.59   |
| 10  | C16   | 623  | VAL  | O-C-N  | -13.04 | 106.27      | 122.57   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | R16   | 1210 | GLU  | O-C-N  | -13.02 | 105.27      | 122.59   |
| 1   | R8    | 1210 | GLU  | O-C-N  | -13.02 | 105.28      | 122.59   |
| 10  | C32   | 623  | VAL  | O-C-N  | -13.01 | 106.31      | 122.57   |
| 2   | M8    | 204  | ILE  | O-C-N  | -13.00 | 109.15      | 121.89   |
| 2   | M16   | 204  | ILE  | O-C-N  | -13.00 | 109.15      | 121.89   |
| 1   | R     | 1210 | GLU  | O-C-N  | -12.99 | 105.32      | 122.59   |
| 18  | B     | 984  | LYS  | O-C-N  | -12.98 | 105.33      | 122.59   |
| 18  | B     | 1363 | ALA  | O-C-N  | -12.97 | 105.34      | 122.59   |
| 2   | M     | 204  | ILE  | O-C-N  | -12.97 | 109.18      | 121.89   |
| 10  | C24   | 623  | VAL  | O-C-N  | -12.94 | 106.40      | 122.57   |
| 20  | E     | 434  | TRP  | O-C-N  | -12.91 | 105.41      | 122.59   |
| 20  | E8    | 434  | TRP  | O-C-N  | -12.90 | 105.44      | 122.59   |
| 13  | V     | 885  | ARG  | O-C-N  | -12.89 | 105.45      | 122.59   |
| 18  | B8    | 1363 | ALA  | O-C-N  | -12.88 | 105.46      | 122.59   |
| 10  | C8    | 250  | GLU  | CA-C-N | -12.87 | 110.84      | 122.29   |
| 10  | C8    | 250  | GLU  | C-N-CA | -12.87 | 110.84      | 122.29   |
| 1   | R     | 1145 | LYS  | CA-C-N | 12.87  | 139.45      | 121.05   |
| 1   | R     | 1145 | LYS  | C-N-CA | 12.87  | 139.45      | 121.05   |
| 1   | R16   | 1145 | LYS  | CA-C-N | 12.86  | 139.44      | 121.05   |
| 1   | R16   | 1145 | LYS  | C-N-CA | 12.86  | 139.44      | 121.05   |
| 10  | C     | 250  | GLU  | CA-C-N | -12.85 | 110.85      | 122.29   |
| 10  | C     | 250  | GLU  | C-N-CA | -12.85 | 110.85      | 122.29   |
| 10  | C16   | 250  | GLU  | CA-C-N | -12.80 | 110.90      | 122.29   |
| 10  | C16   | 250  | GLU  | C-N-CA | -12.80 | 110.90      | 122.29   |
| 1   | R8    | 1145 | LYS  | CA-C-N | 12.80  | 139.35      | 121.05   |
| 1   | R8    | 1145 | LYS  | C-N-CA | 12.80  | 139.35      | 121.05   |
| 10  | C24   | 250  | GLU  | CA-C-N | -12.79 | 110.90      | 122.29   |
| 10  | C24   | 250  | GLU  | C-N-CA | -12.79 | 110.90      | 122.29   |
| 17  | F24   | 79   | ALA  | O-C-N  | -12.79 | 107.72      | 123.06   |
| 10  | C32   | 674  | ASN  | O-C-N  | -12.74 | 103.31      | 122.67   |
| 10  | C16   | 674  | ASN  | O-C-N  | -12.73 | 103.31      | 122.67   |
| 10  | C     | 1068 | THR  | O-C-N  | -12.73 | 105.27      | 122.33   |
| 10  | C     | 674  | ASN  | O-C-N  | -12.72 | 103.33      | 122.67   |
| 19  | 4     | 53   | SER  | O-C-N  | -12.72 | 105.67      | 122.59   |
| 10  | C32   | 250  | GLU  | CA-C-N | -12.72 | 110.96      | 122.29   |
| 10  | C32   | 250  | GLU  | C-N-CA | -12.72 | 110.96      | 122.29   |
| 10  | C24   | 674  | ASN  | O-C-N  | -12.72 | 103.33      | 122.67   |
| 10  | C16   | 1068 | THR  | O-C-N  | -12.72 | 105.28      | 122.33   |
| 19  | 48    | 53   | SER  | O-C-N  | -12.71 | 105.68      | 122.59   |
| 10  | C8    | 674  | ASN  | O-C-N  | -12.70 | 103.37      | 122.67   |
| 10  | C8    | 1068 | THR  | O-C-N  | -12.69 | 105.32      | 122.33   |
| 17  | F8    | 79   | ALA  | O-C-N  | -12.69 | 107.84      | 123.06   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 10  | C32   | 1068 | THR  | O-C-N      | -12.68 | 105.33      | 122.33   |
| 17  | F16   | 79   | ALA  | O-C-N      | -12.68 | 107.84      | 123.06   |
| 10  | C32   | 1509 | SER  | O-C-N      | -12.67 | 108.22      | 123.04   |
| 10  | C     | 1509 | SER  | O-C-N      | -12.65 | 108.24      | 123.04   |
| 10  | C16   | 1509 | SER  | O-C-N      | -12.64 | 108.25      | 123.04   |
| 10  | C24   | 1509 | SER  | O-C-N      | -12.63 | 108.26      | 123.04   |
| 18  | B     | 1118 | LYS  | CA-C-N     | 12.62  | 138.45      | 120.28   |
| 18  | B     | 1118 | LYS  | C-N-CA     | 12.62  | 138.45      | 120.28   |
| 10  | C8    | 1509 | SER  | O-C-N      | -12.61 | 108.29      | 123.04   |
| 10  | C16   | 1663 | SER  | CA-C-N     | 12.61  | 145.62      | 121.54   |
| 10  | C16   | 1663 | SER  | C-N-CA     | 12.61  | 145.62      | 121.54   |
| 10  | C24   | 1068 | THR  | O-C-N      | -12.61 | 105.44      | 122.33   |
| 10  | C24   | 1663 | SER  | CA-C-N     | 12.60  | 145.60      | 121.54   |
| 10  | C24   | 1663 | SER  | C-N-CA     | 12.60  | 145.60      | 121.54   |
| 10  | C     | 1663 | SER  | CA-C-N     | 12.59  | 145.59      | 121.54   |
| 10  | C     | 1663 | SER  | C-N-CA     | 12.59  | 145.59      | 121.54   |
| 10  | C32   | 1663 | SER  | CA-C-N     | 12.58  | 145.57      | 121.54   |
| 10  | C32   | 1663 | SER  | C-N-CA     | 12.58  | 145.57      | 121.54   |
| 6   | O16   | 161  | SER  | O-C-N      | -12.57 | 106.71      | 122.68   |
| 4   | T8    | 386  | HIS  | CG-ND1-CE1 | 12.56  | 130.66      | 109.30   |
| 10  | C32   | 251  | GLY  | CA-C-N     | 12.54  | 145.50      | 121.54   |
| 10  | C32   | 251  | GLY  | C-N-CA     | 12.54  | 145.50      | 121.54   |
| 4   | T     | 386  | HIS  | CG-ND1-CE1 | 12.54  | 130.61      | 109.30   |
| 10  | C24   | 251  | GLY  | CA-C-N     | 12.53  | 145.48      | 121.54   |
| 10  | C24   | 251  | GLY  | C-N-CA     | 12.53  | 145.48      | 121.54   |
| 6   | O     | 161  | SER  | O-C-N      | -12.53 | 106.77      | 122.68   |
| 18  | B8    | 1118 | LYS  | CA-C-N     | 12.53  | 138.32      | 120.28   |
| 18  | B8    | 1118 | LYS  | C-N-CA     | 12.53  | 138.32      | 120.28   |
| 4   | T16   | 386  | HIS  | CG-ND1-CE1 | 12.52  | 130.58      | 109.30   |
| 10  | C16   | 251  | GLY  | CA-C-N     | 12.52  | 145.45      | 121.54   |
| 10  | C16   | 251  | GLY  | C-N-CA     | 12.52  | 145.45      | 121.54   |
| 10  | C     | 251  | GLY  | CA-C-N     | 12.51  | 145.43      | 121.54   |
| 10  | C     | 251  | GLY  | C-N-CA     | 12.51  | 145.43      | 121.54   |
| 20  | E     | 130  | GLY  | O-C-N      | 12.51  | 125.57      | 121.07   |
| 20  | E8    | 420  | LEU  | O-C-N      | -12.51 | 105.96      | 122.59   |
| 6   | O8    | 161  | SER  | O-C-N      | -12.50 | 106.80      | 122.68   |
| 20  | E8    | 130  | GLY  | O-C-N      | 12.49  | 125.57      | 121.07   |
| 10  | C32   | 729  | SER  | O-C-N      | -12.49 | 105.97      | 122.59   |
| 6   | O     | 277  | SER  | O-C-N      | -12.49 | 106.77      | 123.01   |
| 10  | C     | 729  | SER  | O-C-N      | -12.49 | 105.98      | 122.59   |
| 10  | C8    | 251  | GLY  | CA-C-N     | 12.48  | 145.38      | 121.54   |
| 10  | C8    | 251  | GLY  | C-N-CA     | 12.48  | 145.38      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 20  | E     | 38   | PHE  | O-C-N  | -12.48 | 107.00      | 122.35   |
| 6   | O8    | 277  | SER  | O-C-N  | -12.47 | 106.79      | 123.01   |
| 6   | O16   | 277  | SER  | O-C-N  | -12.47 | 106.79      | 123.01   |
| 20  | E     | 420  | LEU  | O-C-N  | -12.47 | 106.00      | 122.59   |
| 10  | C16   | 729  | SER  | O-C-N  | -12.46 | 106.02      | 122.59   |
| 20  | E8    | 38   | PHE  | O-C-N  | -12.46 | 107.03      | 122.35   |
| 13  | V     | 876  | PRO  | O-C-N  | -12.46 | 105.83      | 122.64   |
| 10  | C24   | 729  | SER  | O-C-N  | -12.45 | 106.03      | 122.59   |
| 9   | K     | 1282 | SER  | O-C-N  | -12.44 | 107.02      | 121.32   |
| 9   | K8    | 1282 | SER  | O-C-N  | -12.43 | 107.03      | 121.32   |
| 10  | C     | 1069 | TYR  | CA-C-N | 12.42  | 133.22      | 119.93   |
| 10  | C     | 1069 | TYR  | C-N-CA | 12.42  | 133.22      | 119.93   |
| 19  | 4     | 92   | THR  | O-C-N  | -12.41 | 106.08      | 122.59   |
| 10  | C32   | 248  | LEU  | O-C-N  | -12.41 | 106.09      | 122.59   |
| 19  | 48    | 92   | THR  | O-C-N  | -12.41 | 106.09      | 122.59   |
| 18  | B     | 855  | GLY  | O-C-N  | -12.39 | 106.60      | 122.70   |
| 18  | B8    | 855  | GLY  | O-C-N  | -12.37 | 106.61      | 122.70   |
| 10  | C24   | 248  | LEU  | O-C-N  | -12.37 | 106.14      | 122.59   |
| 10  | C32   | 1069 | TYR  | CA-C-N | 12.37  | 133.17      | 119.93   |
| 10  | C32   | 1069 | TYR  | C-N-CA | 12.37  | 133.17      | 119.93   |
| 9   | K     | 891  | GLU  | O-C-N  | -12.37 | 105.66      | 122.48   |
| 2   | M     | 343  | MET  | O-C-N  | -12.36 | 106.16      | 122.59   |
| 9   | K8    | 891  | GLU  | O-C-N  | -12.36 | 105.68      | 122.48   |
| 10  | C16   | 248  | LEU  | O-C-N  | -12.35 | 106.17      | 122.59   |
| 10  | C8    | 1069 | TYR  | CA-C-N | 12.35  | 133.14      | 119.93   |
| 10  | C8    | 1069 | TYR  | C-N-CA | 12.35  | 133.14      | 119.93   |
| 10  | C     | 248  | LEU  | O-C-N  | -12.34 | 106.18      | 122.59   |
| 2   | M16   | 343  | MET  | O-C-N  | -12.34 | 106.18      | 122.59   |
| 10  | C     | 1503 | VAL  | O-C-N  | -12.34 | 107.15      | 122.57   |
| 10  | C16   | 1503 | VAL  | O-C-N  | -12.34 | 107.15      | 122.57   |
| 9   | K     | 1222 | PHE  | O-C-N  | -12.32 | 108.15      | 122.32   |
| 2   | M8    | 343  | MET  | O-C-N  | -12.32 | 106.20      | 122.59   |
| 10  | C16   | 1069 | TYR  | CA-C-N | 12.32  | 133.11      | 119.93   |
| 10  | C16   | 1069 | TYR  | C-N-CA | 12.32  | 133.11      | 119.93   |
| 10  | C8    | 248  | LEU  | O-C-N  | -12.32 | 106.21      | 122.59   |
| 9   | K8    | 1222 | PHE  | O-C-N  | -12.31 | 108.16      | 122.32   |
| 10  | C8    | 1503 | VAL  | O-C-N  | -12.31 | 107.19      | 122.57   |
| 10  | C32   | 1503 | VAL  | O-C-N  | -12.30 | 107.19      | 122.57   |
| 10  | C24   | 1069 | TYR  | CA-C-N | 12.29  | 133.09      | 119.93   |
| 10  | C24   | 1069 | TYR  | C-N-CA | 12.29  | 133.09      | 119.93   |
| 10  | C24   | 1503 | VAL  | O-C-N  | -12.29 | 107.20      | 122.57   |
| 18  | B     | 1358 | GLU  | O-C-N  | -12.27 | 108.45      | 123.05   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C24   | 1622 | SER  | CA-C-N | 12.25  | 144.01      | 121.97   |
| 10  | C24   | 1622 | SER  | C-N-CA | 12.25  | 144.01      | 121.97   |
| 23  | J24   | 724  | GLY  | O-C-N  | -12.24 | 112.00      | 122.77   |
| 10  | C16   | 1622 | SER  | CA-C-N | 12.24  | 144.00      | 121.97   |
| 10  | C16   | 1622 | SER  | C-N-CA | 12.24  | 144.00      | 121.97   |
| 10  | C8    | 1354 | GLY  | O-C-N  | -12.24 | 106.79      | 122.70   |
| 6   | O8    | 180  | GLY  | O-C-N  | -12.23 | 106.80      | 122.70   |
| 23  | J16   | 724  | GLY  | O-C-N  | -12.23 | 112.01      | 122.77   |
| 6   | O     | 180  | GLY  | O-C-N  | -12.23 | 106.80      | 122.70   |
| 10  | C8    | 1622 | SER  | CA-C-N | 12.23  | 143.98      | 121.97   |
| 10  | C8    | 1622 | SER  | C-N-CA | 12.23  | 143.98      | 121.97   |
| 11  | A16   | 551  | SER  | O-C-N  | -12.22 | 106.34      | 122.59   |
| 10  | C     | 1622 | SER  | CA-C-N | 12.21  | 143.95      | 121.97   |
| 10  | C     | 1622 | SER  | C-N-CA | 12.21  | 143.95      | 121.97   |
| 23  | J32   | 724  | GLY  | O-C-N  | -12.21 | 112.03      | 122.77   |
| 10  | C32   | 1354 | GLY  | O-C-N  | -12.20 | 106.83      | 122.70   |
| 12  | A48   | 551  | SER  | O-C-N  | -12.20 | 106.36      | 122.59   |
| 23  | J8    | 724  | GLY  | O-C-N  | -12.20 | 112.04      | 122.77   |
| 6   | O16   | 180  | GLY  | O-C-N  | -12.19 | 106.85      | 122.70   |
| 10  | C32   | 1622 | SER  | CA-C-N | 12.19  | 143.91      | 121.97   |
| 10  | C32   | 1622 | SER  | C-N-CA | 12.19  | 143.91      | 121.97   |
| 10  | C     | 1354 | GLY  | O-C-N  | -12.19 | 106.86      | 122.70   |
| 11  | A40   | 56   | ALA  | O-C-N  | -12.19 | 107.31      | 121.32   |
| 10  | C24   | 1354 | GLY  | O-C-N  | -12.18 | 106.86      | 122.70   |
| 11  | A16   | 56   | ALA  | O-C-N  | -12.18 | 107.31      | 121.32   |
| 18  | B8    | 1358 | GLU  | O-C-N  | -12.18 | 108.56      | 123.05   |
| 11  | A32   | 56   | ALA  | O-C-N  | -12.17 | 107.32      | 121.32   |
| 11  | A40   | 551  | SER  | O-C-N  | -12.17 | 106.41      | 122.59   |
| 12  | A     | 551  | SER  | O-C-N  | -12.16 | 106.41      | 122.59   |
| 10  | C16   | 1354 | GLY  | O-C-N  | -12.15 | 106.90      | 122.70   |
| 19  | 4     | 54   | LEU  | O-C-N  | -12.15 | 106.43      | 122.59   |
| 11  | A24   | 551  | SER  | O-C-N  | -12.15 | 106.44      | 122.59   |
| 11  | A32   | 551  | SER  | O-C-N  | -12.15 | 106.43      | 122.59   |
| 18  | B     | 413  | ASP  | O-C-N  | -12.14 | 107.82      | 122.63   |
| 10  | C     | 1274 | ALA  | O-C-N  | -12.13 | 106.45      | 122.59   |
| 18  | B8    | 413  | ASP  | O-C-N  | -12.13 | 107.83      | 122.63   |
| 18  | B8    | 1595 | ASP  | O-C-N  | -12.13 | 106.45      | 122.59   |
| 9   | K8    | 1279 | GLU  | O-C-N  | -12.13 | 107.35      | 122.27   |
| 19  | 4     | 66   | ALA  | CA-C-N | 12.12  | 138.56      | 121.71   |
| 19  | 4     | 66   | ALA  | C-N-CA | 12.12  | 138.56      | 121.71   |
| 19  | 48    | 54   | LEU  | O-C-N  | -12.12 | 106.47      | 122.59   |
| 10  | C24   | 1274 | ALA  | O-C-N  | -12.12 | 106.47      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 18  | B     | 1595 | ASP  | O-C-N  | -12.12 | 106.47      | 122.59   |
| 11  | A24   | 56   | ALA  | O-C-N  | -12.12 | 107.39      | 121.32   |
| 18  | B     | 1128 | PRO  | O-C-N  | -12.11 | 106.29      | 122.64   |
| 10  | C32   | 1274 | ALA  | O-C-N  | -12.11 | 106.49      | 122.59   |
| 9   | K     | 1279 | GLU  | O-C-N  | -12.10 | 107.38      | 122.27   |
| 19  | 48    | 66   | ALA  | CA-C-N | 12.10  | 138.52      | 121.71   |
| 19  | 48    | 66   | ALA  | C-N-CA | 12.10  | 138.52      | 121.71   |
| 5   | P8    | 59   | LEU  | O-C-N  | -12.09 | 108.43      | 122.93   |
| 2   | M16   | 344  | GLN  | CA-C-N | -12.08 | 104.23      | 120.54   |
| 2   | M16   | 344  | GLN  | C-N-CA | -12.08 | 104.23      | 120.54   |
| 18  | B8    | 1128 | PRO  | O-C-N  | -12.08 | 106.34      | 122.64   |
| 2   | M8    | 344  | GLN  | CA-C-N | -12.07 | 104.24      | 120.54   |
| 2   | M8    | 344  | GLN  | C-N-CA | -12.07 | 104.24      | 120.54   |
| 5   | P     | 59   | LEU  | O-C-N  | -12.07 | 108.45      | 122.93   |
| 2   | M     | 344  | GLN  | CA-C-N | -12.06 | 104.26      | 120.54   |
| 2   | M     | 344  | GLN  | C-N-CA | -12.06 | 104.26      | 120.54   |
| 10  | C8    | 1274 | ALA  | O-C-N  | -12.06 | 106.55      | 122.59   |
| 10  | C16   | 1274 | ALA  | O-C-N  | -12.05 | 106.56      | 122.59   |
| 14  | W     | 584  | CYS  | O-C-N  | -12.05 | 103.72      | 123.00   |
| 5   | P16   | 59   | LEU  | O-C-N  | -12.04 | 108.49      | 122.93   |
| 5   | P     | 657  | TRP  | CA-C-N | 12.03  | 131.96      | 118.85   |
| 5   | P     | 657  | TRP  | C-N-CA | 12.03  | 131.96      | 118.85   |
| 11  | A32   | 54   | ASN  | O-C-N  | -12.01 | 107.66      | 122.19   |
| 9   | K8    | 728  | GLN  | O-C-N  | -12.00 | 106.64      | 122.59   |
| 5   | P8    | 657  | TRP  | CA-C-N | 11.99  | 131.92      | 118.85   |
| 5   | P8    | 657  | TRP  | C-N-CA | 11.99  | 131.92      | 118.85   |
| 9   | K     | 728  | GLN  | O-C-N  | -11.98 | 106.65      | 122.59   |
| 10  | C     | 283  | SER  | O-C-N  | -11.98 | 106.66      | 122.59   |
| 11  | A24   | 54   | ASN  | O-C-N  | -11.97 | 107.70      | 122.19   |
| 9   | K8    | 1067 | VAL  | O-C-N  | -11.96 | 107.62      | 122.57   |
| 11  | A40   | 54   | ASN  | O-C-N  | -11.96 | 107.71      | 122.19   |
| 21  | H16   | 320  | SER  | O-C-N  | -11.95 | 106.70      | 122.59   |
| 20  | E     | 340  | GLY  | CA-C-N | 11.95  | 139.72      | 120.60   |
| 20  | E     | 340  | GLY  | C-N-CA | 11.95  | 139.72      | 120.60   |
| 9   | K     | 1067 | VAL  | O-C-N  | -11.94 | 107.65      | 122.57   |
| 18  | B     | 1802 | ASP  | O-C-N  | -11.94 | 106.71      | 122.59   |
| 21  | H     | 320  | SER  | O-C-N  | -11.93 | 106.73      | 122.59   |
| 11  | A16   | 54   | ASN  | O-C-N  | -11.93 | 107.76      | 122.19   |
| 18  | B8    | 1802 | ASP  | O-C-N  | -11.92 | 106.74      | 122.59   |
| 20  | E8    | 340  | GLY  | CA-C-N | 11.92  | 139.67      | 120.60   |
| 20  | E8    | 340  | GLY  | C-N-CA | 11.92  | 139.67      | 120.60   |
| 10  | C16   | 283  | SER  | O-C-N  | -11.91 | 106.75      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 5   | P16   | 657  | TRP  | CA-C-N | 11.90  | 131.83      | 118.85   |
| 5   | P16   | 657  | TRP  | C-N-CA | 11.90  | 131.83      | 118.85   |
| 10  | C8    | 283  | SER  | O-C-N  | -11.90 | 106.76      | 122.59   |
| 10  | C24   | 283  | SER  | O-C-N  | -11.90 | 106.77      | 122.59   |
| 10  | C24   | 1061 | ASN  | O-C-N  | -11.90 | 106.77      | 122.59   |
| 21  | H24   | 320  | SER  | O-C-N  | -11.89 | 106.78      | 122.59   |
| 21  | H8    | 320  | SER  | O-C-N  | -11.89 | 106.78      | 122.59   |
| 10  | C32   | 283  | SER  | O-C-N  | -11.89 | 106.78      | 122.59   |
| 6   | O     | 177  | PRO  | CA-C-N | 11.88  | 144.24      | 121.54   |
| 6   | O     | 177  | PRO  | C-N-CA | 11.88  | 144.24      | 121.54   |
| 6   | O8    | 177  | PRO  | CA-C-N | 11.88  | 144.24      | 121.54   |
| 6   | O8    | 177  | PRO  | C-N-CA | 11.88  | 144.24      | 121.54   |
| 6   | O16   | 177  | PRO  | CA-C-N | 11.88  | 144.23      | 121.54   |
| 6   | O16   | 177  | PRO  | C-N-CA | 11.88  | 144.23      | 121.54   |
| 10  | C16   | 1061 | ASN  | O-C-N  | -11.88 | 106.79      | 122.59   |
| 10  | C     | 1061 | ASN  | O-C-N  | -11.88 | 106.79      | 122.59   |
| 18  | B     | 1676 | VAL  | CA-C-N | -11.88 | 104.36      | 120.28   |
| 18  | B     | 1676 | VAL  | C-N-CA | -11.88 | 104.36      | 120.28   |
| 18  | B8    | 1676 | VAL  | CA-C-N | -11.87 | 104.37      | 120.28   |
| 18  | B8    | 1676 | VAL  | C-N-CA | -11.87 | 104.37      | 120.28   |
| 20  | E8    | 345  | LEU  | CA-C-N | -11.86 | 104.60      | 121.20   |
| 20  | E8    | 345  | LEU  | C-N-CA | -11.86 | 104.60      | 121.20   |
| 10  | C32   | 1061 | ASN  | O-C-N  | -11.86 | 106.82      | 122.59   |
| 10  | C8    | 1061 | ASN  | O-C-N  | -11.85 | 106.83      | 122.59   |
| 20  | E8    | 341  | TYR  | O-C-N  | -11.85 | 106.99      | 122.39   |
| 20  | E     | 345  | LEU  | CA-C-N | -11.85 | 104.61      | 121.20   |
| 20  | E     | 345  | LEU  | C-N-CA | -11.85 | 104.61      | 121.20   |
| 10  | C     | 1077 | ALA  | CA-C-N | 11.85  | 144.63      | 121.41   |
| 10  | C     | 1077 | ALA  | C-N-CA | 11.85  | 144.63      | 121.41   |
| 10  | C24   | 1077 | ALA  | CA-C-N | 11.84  | 144.62      | 121.41   |
| 10  | C24   | 1077 | ALA  | C-N-CA | 11.84  | 144.62      | 121.41   |
| 2   | M8    | 344  | GLN  | O-C-N  | -11.84 | 106.85      | 122.59   |
| 10  | C16   | 1077 | ALA  | CA-C-N | 11.84  | 144.61      | 121.41   |
| 10  | C16   | 1077 | ALA  | C-N-CA | 11.84  | 144.61      | 121.41   |
| 10  | C32   | 1077 | ALA  | CA-C-N | 11.83  | 144.60      | 121.41   |
| 10  | C32   | 1077 | ALA  | C-N-CA | 11.83  | 144.60      | 121.41   |
| 20  | E     | 422  | SER  | O-C-N  | -11.83 | 111.68      | 121.38   |
| 2   | M     | 344  | GLN  | O-C-N  | -11.83 | 106.86      | 122.59   |
| 10  | C8    | 1077 | ALA  | CA-C-N | 11.83  | 144.59      | 121.41   |
| 10  | C8    | 1077 | ALA  | C-N-CA | 11.83  | 144.59      | 121.41   |
| 20  | E8    | 422  | SER  | O-C-N  | -11.82 | 111.69      | 121.38   |
| 20  | E     | 341  | TYR  | O-C-N  | -11.81 | 107.04      | 122.39   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 2   | M16   | 344  | GLN  | O-C-N  | -11.81 | 106.88      | 122.59   |
| 13  | V     | 820  | ASP  | O-C-N  | -11.81 | 108.67      | 122.84   |
| 10  | C32   | 1355 | GLU  | O-C-N  | -11.80 | 106.90      | 122.59   |
| 10  | C16   | 1033 | GLY  | O-C-N  | -11.78 | 109.37      | 122.68   |
| 10  | C24   | 336  | THR  | O-C-N  | -11.78 | 109.31      | 122.03   |
| 10  | C     | 1355 | GLU  | O-C-N  | -11.77 | 106.94      | 122.59   |
| 10  | C16   | 1355 | GLU  | O-C-N  | -11.76 | 106.95      | 122.59   |
| 10  | C8    | 1033 | GLY  | O-C-N  | -11.74 | 109.41      | 122.68   |
| 10  | C32   | 1033 | GLY  | O-C-N  | -11.74 | 109.42      | 122.68   |
| 18  | B8    | 508  | ALA  | CA-C-N | 11.73  | 143.94      | 121.54   |
| 18  | B8    | 508  | ALA  | C-N-CA | 11.73  | 143.94      | 121.54   |
| 9   | K     | 1140 | GLN  | O-C-N  | -11.72 | 107.00      | 122.59   |
| 10  | C     | 1033 | GLY  | O-C-N  | -11.72 | 109.43      | 122.68   |
| 9   | K8    | 1140 | GLN  | O-C-N  | -11.72 | 107.00      | 122.59   |
| 18  | B     | 508  | ALA  | CA-C-N | 11.72  | 143.92      | 121.54   |
| 18  | B     | 508  | ALA  | C-N-CA | 11.72  | 143.92      | 121.54   |
| 19  | 4     | 68   | GLY  | CA-C-N | 11.72  | 143.92      | 121.54   |
| 19  | 4     | 68   | GLY  | C-N-CA | 11.72  | 143.92      | 121.54   |
| 19  | 48    | 68   | GLY  | CA-C-N | 11.71  | 143.91      | 121.54   |
| 19  | 48    | 68   | GLY  | C-N-CA | 11.71  | 143.91      | 121.54   |
| 10  | C24   | 1355 | GLU  | O-C-N  | -11.71 | 107.02      | 122.59   |
| 20  | E8    | 436  | THR  | CA-C-N | 11.70  | 143.89      | 121.54   |
| 20  | E8    | 436  | THR  | C-N-CA | 11.70  | 143.89      | 121.54   |
| 20  | E     | 436  | THR  | CA-C-N | 11.70  | 143.88      | 121.54   |
| 20  | E     | 436  | THR  | C-N-CA | 11.70  | 143.88      | 121.54   |
| 18  | B     | 1111 | LYS  | CA-C-N | 11.69  | 137.55      | 120.83   |
| 18  | B     | 1111 | LYS  | C-N-CA | 11.69  | 137.55      | 120.83   |
| 10  | C16   | 336  | THR  | O-C-N  | -11.68 | 109.42      | 122.03   |
| 9   | K8    | 930  | THR  | O-C-N  | -11.68 | 109.23      | 123.01   |
| 18  | B8    | 1111 | LYS  | CA-C-N | 11.68  | 137.53      | 120.83   |
| 18  | B8    | 1111 | LYS  | C-N-CA | 11.68  | 137.53      | 120.83   |
| 14  | W     | 600  | PRO  | O-C-N  | -11.67 | 106.88      | 122.64   |
| 10  | C8    | 1355 | GLU  | O-C-N  | -11.67 | 107.07      | 122.59   |
| 18  | B8    | 611  | ASN  | O-C-N  | -11.65 | 107.10      | 122.59   |
| 18  | B     | 1129 | LYS  | O-C-N  | -11.64 | 107.11      | 122.59   |
| 10  | C8    | 336  | THR  | O-C-N  | -11.64 | 109.46      | 122.03   |
| 18  | B8    | 1129 | LYS  | O-C-N  | -11.63 | 107.11      | 122.59   |
| 10  | C24   | 1033 | GLY  | O-C-N  | -11.62 | 109.54      | 122.68   |
| 18  | B     | 611  | ASN  | O-C-N  | -11.62 | 107.14      | 122.59   |
| 9   | K     | 930  | THR  | O-C-N  | -11.59 | 109.33      | 123.01   |
| 18  | B     | 1119 | LYS  | CA-C-N | -11.56 | 99.45       | 121.54   |
| 18  | B     | 1119 | LYS  | C-N-CA | -11.56 | 99.45       | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C32   | 336  | THR  | O-C-N  | -11.56 | 109.54      | 122.03   |
| 10  | C     | 336  | THR  | O-C-N  | -11.56 | 109.54      | 122.03   |
| 18  | B8    | 1119 | LYS  | CA-C-N | -11.55 | 99.47       | 121.54   |
| 18  | B8    | 1119 | LYS  | C-N-CA | -11.55 | 99.47       | 121.54   |
| 10  | C24   | 1129 | VAL  | CA-C-N | 11.53  | 143.56      | 121.54   |
| 10  | C24   | 1129 | VAL  | C-N-CA | 11.53  | 143.56      | 121.54   |
| 10  | C     | 1129 | VAL  | CA-C-N | 11.52  | 143.55      | 121.54   |
| 10  | C     | 1129 | VAL  | C-N-CA | 11.52  | 143.55      | 121.54   |
| 10  | C32   | 1129 | VAL  | CA-C-N | 11.50  | 143.51      | 121.54   |
| 10  | C32   | 1129 | VAL  | C-N-CA | 11.50  | 143.51      | 121.54   |
| 10  | C8    | 1129 | VAL  | CA-C-N | 11.49  | 143.49      | 121.54   |
| 10  | C8    | 1129 | VAL  | C-N-CA | 11.49  | 143.49      | 121.54   |
| 10  | C16   | 1129 | VAL  | CA-C-N | 11.49  | 143.48      | 121.54   |
| 10  | C16   | 1129 | VAL  | C-N-CA | 11.49  | 143.48      | 121.54   |
| 19  | 48    | 72   | GLY  | CA-C-N | 11.45  | 143.41      | 121.54   |
| 19  | 48    | 72   | GLY  | C-N-CA | 11.45  | 143.41      | 121.54   |
| 19  | 4     | 72   | GLY  | CA-C-N | 11.44  | 143.40      | 121.54   |
| 19  | 4     | 72   | GLY  | C-N-CA | 11.44  | 143.40      | 121.54   |
| 20  | E8    | 204  | SER  | O-C-N  | -11.39 | 109.22      | 122.20   |
| 20  | E     | 204  | SER  | O-C-N  | -11.38 | 109.22      | 122.20   |
| 18  | B8    | 1604 | ASN  | O-C-N  | -11.36 | 107.48      | 122.59   |
| 20  | E     | 438  | SER  | O-C-N  | -11.35 | 107.49      | 122.59   |
| 18  | B     | 1604 | ASN  | O-C-N  | -11.31 | 107.54      | 122.59   |
| 10  | C24   | 717  | GLU  | O-C-N  | -11.30 | 108.36      | 122.27   |
| 20  | E8    | 438  | SER  | O-C-N  | -11.30 | 107.56      | 122.59   |
| 10  | C16   | 717  | GLU  | O-C-N  | -11.26 | 108.42      | 122.27   |
| 10  | C32   | 717  | GLU  | O-C-N  | -11.26 | 108.42      | 122.27   |
| 7   | Q16   | 57   | ASN  | O-C-N  | 11.24  | 131.49      | 121.37   |
| 18  | B8    | 1131 | THR  | O-C-N  | -11.24 | 107.64      | 122.59   |
| 7   | Q     | 57   | ASN  | O-C-N  | 11.23  | 131.48      | 121.37   |
| 10  | C     | 632  | GLN  | CA-C-N | 11.23  | 142.99      | 121.54   |
| 10  | C     | 632  | GLN  | C-N-CA | 11.23  | 142.99      | 121.54   |
| 17  | F     | 79   | ALA  | O-C-N  | -11.21 | 107.72      | 123.07   |
| 10  | C     | 717  | GLU  | O-C-N  | -11.21 | 108.49      | 122.27   |
| 18  | B     | 1131 | THR  | O-C-N  | -11.21 | 107.69      | 122.59   |
| 2   | M8    | 386  | ASN  | O-C-N  | -11.19 | 107.70      | 122.59   |
| 10  | C32   | 632  | GLN  | CA-C-N | 11.19  | 142.90      | 121.54   |
| 10  | C32   | 632  | GLN  | C-N-CA | 11.19  | 142.90      | 121.54   |
| 7   | Q8    | 57   | ASN  | O-C-N  | 11.18  | 131.44      | 121.37   |
| 2   | M     | 386  | ASN  | O-C-N  | -11.18 | 107.72      | 122.59   |
| 10  | C16   | 632  | GLN  | CA-C-N | 11.18  | 142.89      | 121.54   |
| 10  | C16   | 632  | GLN  | C-N-CA | 11.18  | 142.89      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C24   | 632  | GLN  | CA-C-N | 11.15  | 142.84      | 121.54   |
| 10  | C24   | 632  | GLN  | C-N-CA | 11.15  | 142.84      | 121.54   |
| 10  | C     | 635  | GLN  | CA-C-N | 11.15  | 137.90      | 121.18   |
| 10  | C     | 635  | GLN  | C-N-CA | 11.15  | 137.90      | 121.18   |
| 23  | J24   | 681  | GLU  | CA-C-N | -11.14 | 106.82      | 122.87   |
| 23  | J24   | 681  | GLU  | C-N-CA | -11.14 | 106.82      | 122.87   |
| 9   | K8    | 1272 | GLU  | O-C-N  | -11.13 | 109.72      | 122.75   |
| 2   | M16   | 386  | ASN  | O-C-N  | -11.13 | 107.79      | 122.59   |
| 23  | J16   | 681  | GLU  | CA-C-N | -11.13 | 106.84      | 122.87   |
| 23  | J16   | 681  | GLU  | C-N-CA | -11.13 | 106.84      | 122.87   |
| 10  | C16   | 635  | GLN  | CA-C-N | 11.12  | 137.87      | 121.18   |
| 10  | C16   | 635  | GLN  | C-N-CA | 11.12  | 137.87      | 121.18   |
| 23  | J32   | 681  | GLU  | CA-C-N | -11.12 | 106.85      | 122.87   |
| 23  | J32   | 681  | GLU  | C-N-CA | -11.12 | 106.85      | 122.87   |
| 9   | K     | 1272 | GLU  | O-C-N  | -11.12 | 109.74      | 122.75   |
| 10  | C24   | 673  | VAL  | O-C-N  | -11.12 | 107.13      | 122.59   |
| 18  | B8    | 974  | SER  | O-C-N  | -11.12 | 110.62      | 122.07   |
| 10  | C32   | 635  | GLN  | CA-C-N | 11.12  | 137.85      | 121.18   |
| 10  | C32   | 635  | GLN  | C-N-CA | 11.12  | 137.85      | 121.18   |
| 10  | C     | 673  | VAL  | O-C-N  | -11.11 | 107.15      | 122.59   |
| 23  | J8    | 681  | GLU  | CA-C-N | -11.11 | 106.87      | 122.87   |
| 23  | J8    | 681  | GLU  | C-N-CA | -11.11 | 106.87      | 122.87   |
| 10  | C32   | 1622 | SER  | O-C-N  | -11.11 | 107.82      | 122.59   |
| 10  | C24   | 635  | GLN  | CA-C-N | 11.10  | 137.82      | 121.18   |
| 10  | C24   | 635  | GLN  | C-N-CA | 11.10  | 137.82      | 121.18   |
| 10  | C24   | 337  | ILE  | O-C-N  | -11.09 | 108.70      | 122.57   |
| 10  | C8    | 673  | VAL  | O-C-N  | -11.09 | 107.17      | 122.59   |
| 10  | C32   | 1055 | GLU  | O-C-N  | -11.09 | 107.84      | 122.59   |
| 10  | C32   | 673  | VAL  | O-C-N  | -11.08 | 107.19      | 122.59   |
| 10  | C24   | 1622 | SER  | O-C-N  | -11.07 | 107.86      | 122.59   |
| 10  | C24   | 1055 | GLU  | O-C-N  | -11.07 | 107.87      | 122.59   |
| 18  | B     | 974  | SER  | O-C-N  | -11.07 | 110.67      | 122.07   |
| 10  | C24   | 634  | SER  | O-C-N  | -11.06 | 107.87      | 122.59   |
| 10  | C     | 1055 | GLU  | O-C-N  | -11.06 | 107.88      | 122.59   |
| 10  | C16   | 673  | VAL  | O-C-N  | -11.05 | 107.23      | 122.59   |
| 10  | C8    | 1055 | GLU  | O-C-N  | -11.05 | 107.89      | 122.59   |
| 10  | C16   | 1622 | SER  | O-C-N  | -11.05 | 107.89      | 122.59   |
| 18  | B     | 1668 | PHE  | O-C-N  | -11.04 | 109.71      | 121.42   |
| 18  | B     | 688  | GLY  | O-C-N  | -11.03 | 108.36      | 122.70   |
| 18  | B8    | 1668 | PHE  | O-C-N  | -11.03 | 109.73      | 121.42   |
| 10  | C32   | 337  | ILE  | O-C-N  | -11.02 | 108.80      | 122.57   |
| 9   | K8    | 724  | GLY  | CA-C-N | 11.02  | 142.58      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 9   | K8    | 724  | GLY  | C-N-CA | 11.02  | 142.58      | 121.54   |
| 10  | C16   | 337  | ILE  | O-C-N  | -11.02 | 108.80      | 122.57   |
| 18  | B8    | 1747 | SER  | CA-C-N | -11.02 | 104.94      | 122.23   |
| 18  | B8    | 1747 | SER  | C-N-CA | -11.02 | 104.94      | 122.23   |
| 10  | C16   | 1055 | GLU  | O-C-N  | -11.01 | 107.94      | 122.59   |
| 10  | C     | 337  | ILE  | O-C-N  | -11.01 | 108.81      | 122.57   |
| 18  | B     | 1747 | SER  | CA-C-N | -11.01 | 104.94      | 122.23   |
| 18  | B     | 1747 | SER  | C-N-CA | -11.01 | 104.94      | 122.23   |
| 10  | C8    | 1622 | SER  | O-C-N  | -11.00 | 107.96      | 122.59   |
| 10  | C8    | 337  | ILE  | O-C-N  | -11.00 | 108.82      | 122.57   |
| 18  | B8    | 688  | GLY  | O-C-N  | -11.00 | 108.41      | 122.70   |
| 10  | C16   | 634  | SER  | O-C-N  | -10.99 | 107.97      | 122.59   |
| 10  | C     | 634  | SER  | O-C-N  | -10.98 | 107.98      | 122.59   |
| 10  | C     | 1622 | SER  | O-C-N  | -10.98 | 107.99      | 122.59   |
| 10  | C16   | 619  | LEU  | CA-C-N | 10.97  | 133.55      | 119.84   |
| 10  | C16   | 619  | LEU  | C-N-CA | 10.97  | 133.55      | 119.84   |
| 10  | C32   | 619  | LEU  | CA-C-N | 10.97  | 133.56      | 119.84   |
| 10  | C32   | 619  | LEU  | C-N-CA | 10.97  | 133.56      | 119.84   |
| 9   | K     | 724  | GLY  | CA-C-N | 10.96  | 142.48      | 121.54   |
| 9   | K     | 724  | GLY  | C-N-CA | 10.96  | 142.48      | 121.54   |
| 17  | F8    | 73   | GLY  | CA-C-N | -10.96 | 102.23      | 121.97   |
| 17  | F8    | 73   | GLY  | C-N-CA | -10.96 | 102.23      | 121.97   |
| 17  | F24   | 73   | GLY  | CA-C-N | -10.97 | 102.23      | 121.97   |
| 17  | F24   | 73   | GLY  | C-N-CA | -10.97 | 102.23      | 121.97   |
| 7   | Q16   | 144  | GLU  | O-C-N  | -10.96 | 107.97      | 122.77   |
| 17  | F     | 73   | GLY  | CA-C-N | -10.96 | 102.25      | 121.97   |
| 17  | F     | 73   | GLY  | C-N-CA | -10.96 | 102.25      | 121.97   |
| 17  | F16   | 73   | GLY  | CA-C-N | -10.95 | 102.25      | 121.97   |
| 17  | F16   | 73   | GLY  | C-N-CA | -10.95 | 102.25      | 121.97   |
| 10  | C24   | 619  | LEU  | CA-C-N | 10.95  | 133.53      | 119.84   |
| 10  | C24   | 619  | LEU  | C-N-CA | 10.95  | 133.53      | 119.84   |
| 10  | C8    | 619  | LEU  | CA-C-N | 10.94  | 133.52      | 119.84   |
| 10  | C8    | 619  | LEU  | C-N-CA | 10.94  | 133.52      | 119.84   |
| 10  | C32   | 634  | SER  | O-C-N  | -10.93 | 108.05      | 122.59   |
| 15  | J     | 687  | SER  | O-C-N  | -10.93 | 111.58      | 121.30   |
| 7   | Q8    | 144  | GLU  | O-C-N  | -10.91 | 108.03      | 122.77   |
| 9   | K     | 638  | TRP  | O-C-N  | -10.90 | 108.09      | 122.59   |
| 7   | Q     | 144  | GLU  | O-C-N  | -10.90 | 108.06      | 122.77   |
| 10  | C     | 619  | LEU  | CA-C-N | 10.89  | 133.45      | 119.84   |
| 10  | C     | 619  | LEU  | C-N-CA | 10.89  | 133.45      | 119.84   |
| 10  | C8    | 675  | ASP  | O-C-N  | -10.88 | 108.86      | 122.68   |
| 10  | C24   | 675  | ASP  | O-C-N  | -10.88 | 108.86      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 9   | K8    | 638  | TRP  | O-C-N  | -10.85 | 108.16      | 122.59   |
| 20  | E8    | 202  | ASP  | O-C-N  | -10.81 | 108.21      | 122.59   |
| 10  | C     | 675  | ASP  | O-C-N  | -10.80 | 108.96      | 122.68   |
| 3   | N     | 2    | PRO  | O-C-N  | -10.79 | 111.22      | 122.98   |
| 2   | M8    | 759  | LEU  | O-C-N  | -10.78 | 108.25      | 122.59   |
| 10  | C32   | 675  | ASP  | O-C-N  | -10.78 | 108.99      | 122.68   |
| 3   | N16   | 2    | PRO  | O-C-N  | -10.77 | 111.25      | 122.98   |
| 20  | E     | 202  | ASP  | O-C-N  | -10.77 | 108.27      | 122.59   |
| 10  | C16   | 675  | ASP  | O-C-N  | -10.76 | 109.01      | 122.68   |
| 2   | M16   | 759  | LEU  | O-C-N  | -10.76 | 108.28      | 122.59   |
| 9   | K8    | 1220 | ASN  | O-C-N  | -10.74 | 108.30      | 122.59   |
| 5   | P16   | 161  | ASN  | O-C-N  | -10.74 | 108.31      | 122.59   |
| 10  | C16   | 1128 | SER  | CA-C-N | 10.74  | 141.30      | 121.97   |
| 10  | C16   | 1128 | SER  | C-N-CA | 10.74  | 141.30      | 121.97   |
| 10  | C8    | 1128 | SER  | CA-C-N | 10.73  | 141.29      | 121.97   |
| 10  | C8    | 1128 | SER  | C-N-CA | 10.73  | 141.29      | 121.97   |
| 9   | K     | 1220 | ASN  | O-C-N  | -10.73 | 108.32      | 122.59   |
| 10  | C24   | 1128 | SER  | CA-C-N | 10.73  | 141.28      | 121.97   |
| 10  | C24   | 1128 | SER  | C-N-CA | 10.73  | 141.28      | 121.97   |
| 2   | M     | 759  | LEU  | O-C-N  | -10.72 | 108.33      | 122.59   |
| 10  | C     | 1128 | SER  | CA-C-N | 10.72  | 141.27      | 121.97   |
| 10  | C     | 1128 | SER  | C-N-CA | 10.72  | 141.27      | 121.97   |
| 5   | P8    | 161  | ASN  | O-C-N  | -10.72 | 108.33      | 122.59   |
| 5   | P     | 161  | ASN  | O-C-N  | -10.72 | 108.34      | 122.59   |
| 10  | C32   | 1128 | SER  | CA-C-N | 10.71  | 141.24      | 121.97   |
| 10  | C32   | 1128 | SER  | C-N-CA | 10.71  | 141.24      | 121.97   |
| 3   | N8    | 2    | PRO  | O-C-N  | -10.70 | 111.32      | 122.98   |
| 10  | C24   | 337  | ILE  | CA-C-N | 10.70  | 134.34      | 120.44   |
| 10  | C24   | 337  | ILE  | C-N-CA | 10.70  | 134.34      | 120.44   |
| 5   | P     | 143  | ASN  | O-C-N  | -10.68 | 107.34      | 122.29   |
| 5   | P8    | 143  | ASN  | O-C-N  | -10.67 | 107.35      | 122.29   |
| 11  | A24   | 470  | LEU  | O-C-N  | -10.67 | 108.39      | 122.59   |
| 11  | A16   | 470  | LEU  | O-C-N  | -10.67 | 108.40      | 122.59   |
| 12  | A48   | 470  | LEU  | O-C-N  | -10.67 | 108.40      | 122.59   |
| 5   | P     | 10   | GLY  | O-C-N  | -10.66 | 108.84      | 122.70   |
| 18  | B     | 1808 | GLY  | O-C-N  | -10.65 | 108.85      | 122.70   |
| 10  | C16   | 337  | ILE  | CA-C-N | 10.65  | 134.29      | 120.44   |
| 10  | C16   | 337  | ILE  | C-N-CA | 10.65  | 134.29      | 120.44   |
| 18  | B8    | 1808 | GLY  | O-C-N  | -10.64 | 108.86      | 122.70   |
| 10  | C24   | 1440 | SER  | O-C-N  | -10.64 | 108.59      | 122.43   |
| 10  | C32   | 447  | PHE  | CA-C-N | 10.64  | 141.87      | 121.54   |
| 10  | C32   | 447  | PHE  | C-N-CA | 10.64  | 141.87      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 5   | P16   | 143  | ASN  | O-C-N  | -10.64 | 107.39      | 122.29   |
| 10  | C32   | 1440 | SER  | O-C-N  | -10.64 | 108.60      | 122.43   |
| 11  | A32   | 470  | LEU  | O-C-N  | -10.63 | 108.45      | 122.59   |
| 12  | A     | 470  | LEU  | O-C-N  | -10.63 | 108.45      | 122.59   |
| 2   | M8    | 351  | ALA  | O-C-N  | -10.63 | 108.46      | 122.59   |
| 9   | K     | 1052 | SER  | O-C-N  | -10.63 | 108.46      | 122.59   |
| 5   | P8    | 10   | GLY  | O-C-N  | -10.62 | 108.89      | 122.70   |
| 10  | C16   | 1440 | SER  | O-C-N  | -10.62 | 108.62      | 122.43   |
| 10  | C8    | 337  | ILE  | CA-C-N | 10.62  | 134.24      | 120.44   |
| 10  | C8    | 337  | ILE  | C-N-CA | 10.62  | 134.24      | 120.44   |
| 14  | W     | 598  | ILE  | O-C-N  | -10.62 | 109.30      | 122.57   |
| 10  | C8    | 1440 | SER  | O-C-N  | -10.62 | 108.63      | 122.43   |
| 10  | C     | 337  | ILE  | CA-C-N | 10.61  | 134.23      | 120.44   |
| 10  | C     | 337  | ILE  | C-N-CA | 10.61  | 134.23      | 120.44   |
| 10  | C16   | 1785 | SER  | O-C-N  | -10.60 | 107.35      | 122.41   |
| 2   | M16   | 351  | ALA  | O-C-N  | -10.60 | 108.49      | 122.59   |
| 2   | M     | 351  | ALA  | O-C-N  | -10.60 | 108.50      | 122.59   |
| 10  | C16   | 447  | PHE  | CA-C-N | 10.59  | 141.77      | 121.54   |
| 10  | C16   | 447  | PHE  | C-N-CA | 10.59  | 141.77      | 121.54   |
| 10  | C     | 1785 | SER  | O-C-N  | -10.59 | 107.37      | 122.41   |
| 5   | P16   | 10   | GLY  | O-C-N  | -10.59 | 108.94      | 122.70   |
| 9   | K8    | 1052 | SER  | O-C-N  | -10.59 | 108.51      | 122.59   |
| 10  | C32   | 337  | ILE  | CA-C-N | 10.59  | 134.21      | 120.44   |
| 10  | C32   | 337  | ILE  | C-N-CA | 10.59  | 134.21      | 120.44   |
| 10  | C24   | 1785 | SER  | O-C-N  | -10.59 | 107.37      | 122.41   |
| 10  | C16   | 1072 | ASP  | CA-C-N | 10.59  | 131.29      | 120.60   |
| 10  | C16   | 1072 | ASP  | C-N-CA | 10.59  | 131.29      | 120.60   |
| 11  | A40   | 470  | LEU  | O-C-N  | -10.59 | 108.51      | 122.59   |
| 10  | C32   | 1785 | SER  | O-C-N  | -10.58 | 107.39      | 122.41   |
| 10  | C24   | 447  | PHE  | CA-C-N | 10.57  | 141.73      | 121.54   |
| 10  | C24   | 447  | PHE  | C-N-CA | 10.57  | 141.73      | 121.54   |
| 10  | C8    | 1785 | SER  | O-C-N  | -10.56 | 107.41      | 122.41   |
| 1   | R     | 1201 | LEU  | CA-C-N | -10.55 | 106.72      | 120.65   |
| 1   | R     | 1201 | LEU  | C-N-CA | -10.55 | 106.72      | 120.65   |
| 10  | C     | 1072 | ASP  | CA-C-N | 10.55  | 131.26      | 120.60   |
| 10  | C     | 1072 | ASP  | C-N-CA | 10.55  | 131.26      | 120.60   |
| 1   | R16   | 1201 | LEU  | CA-C-N | -10.54 | 106.74      | 120.65   |
| 1   | R16   | 1201 | LEU  | C-N-CA | -10.54 | 106.74      | 120.65   |
| 10  | C24   | 1072 | ASP  | CA-C-N | 10.54  | 131.24      | 120.60   |
| 10  | C24   | 1072 | ASP  | C-N-CA | 10.54  | 131.24      | 120.60   |
| 10  | C     | 1440 | SER  | O-C-N  | -10.54 | 108.73      | 122.43   |
| 7   | Q16   | 90   | GLY  | O-C-N  | -10.53 | 109.01      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C32   | 1072 | ASP  | CA-C-N | 10.53  | 131.23      | 120.60   |
| 10  | C32   | 1072 | ASP  | C-N-CA | 10.53  | 131.23      | 120.60   |
| 1   | R8    | 1201 | LEU  | CA-C-N | -10.51 | 106.78      | 120.65   |
| 1   | R8    | 1201 | LEU  | C-N-CA | -10.51 | 106.78      | 120.65   |
| 18  | B8    | 192  | PRO  | CA-C-N | 10.50  | 141.60      | 121.54   |
| 18  | B8    | 192  | PRO  | C-N-CA | 10.50  | 141.60      | 121.54   |
| 10  | C32   | 1059 | ALA  | O-C-N  | -10.50 | 111.11      | 122.03   |
| 10  | C24   | 1446 | HIS  | CA-C-N | 10.49  | 134.70      | 120.54   |
| 10  | C24   | 1446 | HIS  | C-N-CA | 10.49  | 134.70      | 120.54   |
| 10  | C24   | 1059 | ALA  | O-C-N  | -10.48 | 111.13      | 122.03   |
| 10  | C8    | 1072 | ASP  | CA-C-N | 10.48  | 131.19      | 120.60   |
| 10  | C8    | 1072 | ASP  | C-N-CA | 10.48  | 131.19      | 120.60   |
| 10  | C8    | 1446 | HIS  | CA-C-N | 10.48  | 134.69      | 120.54   |
| 10  | C8    | 1446 | HIS  | C-N-CA | 10.48  | 134.69      | 120.54   |
| 7   | Q8    | 90   | GLY  | O-C-N  | -10.48 | 109.08      | 122.70   |
| 18  | B     | 192  | PRO  | CA-C-N | 10.48  | 141.55      | 121.54   |
| 18  | B     | 192  | PRO  | C-N-CA | 10.48  | 141.55      | 121.54   |
| 23  | J32   | 738  | MET  | CA-C-N | -10.46 | 102.87      | 121.70   |
| 23  | J32   | 738  | MET  | C-N-CA | -10.46 | 102.87      | 121.70   |
| 23  | J8    | 738  | MET  | CA-C-N | -10.46 | 102.87      | 121.70   |
| 23  | J8    | 738  | MET  | C-N-CA | -10.46 | 102.87      | 121.70   |
| 23  | J16   | 738  | MET  | CA-C-N | -10.46 | 102.87      | 121.70   |
| 23  | J16   | 738  | MET  | C-N-CA | -10.46 | 102.87      | 121.70   |
| 7   | Q     | 90   | GLY  | O-C-N  | -10.46 | 109.10      | 122.70   |
| 10  | C16   | 1059 | ALA  | O-C-N  | -10.45 | 111.16      | 122.03   |
| 10  | C     | 1446 | HIS  | CA-C-N | 10.45  | 134.65      | 120.54   |
| 10  | C     | 1446 | HIS  | C-N-CA | 10.45  | 134.65      | 120.54   |
| 10  | C     | 1059 | ALA  | O-C-N  | -10.45 | 111.16      | 122.03   |
| 23  | J8    | 679  | GLU  | O-C-N  | -10.44 | 107.67      | 122.29   |
| 23  | J24   | 738  | MET  | CA-C-N | -10.44 | 102.91      | 121.70   |
| 23  | J24   | 738  | MET  | C-N-CA | -10.44 | 102.91      | 121.70   |
| 23  | J32   | 679  | GLU  | O-C-N  | -10.43 | 107.69      | 122.29   |
| 10  | C32   | 1446 | HIS  | CA-C-N | 10.43  | 134.62      | 120.54   |
| 10  | C32   | 1446 | HIS  | C-N-CA | 10.43  | 134.62      | 120.54   |
| 10  | C16   | 1446 | HIS  | CA-C-N | 10.42  | 134.61      | 120.54   |
| 10  | C16   | 1446 | HIS  | C-N-CA | 10.42  | 134.61      | 120.54   |
| 10  | C8    | 1059 | ALA  | O-C-N  | -10.42 | 111.19      | 122.03   |
| 9   | K     | 1193 | SER  | CA-C-N | 10.42  | 134.65      | 120.38   |
| 9   | K     | 1193 | SER  | C-N-CA | 10.42  | 134.65      | 120.38   |
| 9   | K     | 718  | PHE  | O-C-N  | -10.41 | 108.90      | 122.43   |
| 10  | C24   | 1067 | SER  | CA-C-N | 10.40  | 138.37      | 120.68   |
| 10  | C24   | 1067 | SER  | C-N-CA | 10.40  | 138.37      | 120.68   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 19  | 4     | 65   | LYS  | CA-C-N | -10.40 | 101.67      | 121.54   |
| 19  | 4     | 65   | LYS  | C-N-CA | -10.40 | 101.67      | 121.54   |
| 19  | 48    | 65   | LYS  | CA-C-N | -10.39 | 101.69      | 121.54   |
| 19  | 48    | 65   | LYS  | C-N-CA | -10.39 | 101.69      | 121.54   |
| 23  | J24   | 679  | GLU  | O-C-N  | -10.39 | 107.74      | 122.29   |
| 23  | J16   | 679  | GLU  | O-C-N  | -10.39 | 107.74      | 122.29   |
| 10  | C8    | 1540 | GLU  | O-C-N  | -10.39 | 109.72      | 122.71   |
| 10  | C     | 1067 | SER  | CA-C-N | 10.38  | 138.33      | 120.68   |
| 10  | C     | 1067 | SER  | C-N-CA | 10.38  | 138.33      | 120.68   |
| 18  | B8    | 1121 | ALA  | CA-C-N | -10.38 | 101.70      | 121.54   |
| 18  | B8    | 1121 | ALA  | C-N-CA | -10.38 | 101.70      | 121.54   |
| 18  | B     | 1121 | ALA  | CA-C-N | -10.38 | 101.71      | 121.54   |
| 18  | B     | 1121 | ALA  | C-N-CA | -10.38 | 101.71      | 121.54   |
| 10  | C32   | 1067 | SER  | CA-C-N | 10.38  | 138.32      | 120.68   |
| 10  | C32   | 1067 | SER  | C-N-CA | 10.38  | 138.32      | 120.68   |
| 2   | M16   | 156  | GLY  | CA-C-N | 10.37  | 141.74      | 121.41   |
| 2   | M16   | 156  | GLY  | C-N-CA | 10.37  | 141.74      | 121.41   |
| 10  | C16   | 1067 | SER  | CA-C-N | 10.37  | 138.31      | 120.68   |
| 10  | C16   | 1067 | SER  | C-N-CA | 10.37  | 138.31      | 120.68   |
| 10  | C8    | 1067 | SER  | CA-C-N | 10.37  | 138.31      | 120.68   |
| 10  | C8    | 1067 | SER  | C-N-CA | 10.37  | 138.31      | 120.68   |
| 9   | K     | 1193 | SER  | O-C-N  | -10.36 | 110.62      | 122.75   |
| 18  | B8    | 978  | ASN  | O-C-N  | -10.36 | 111.40      | 122.07   |
| 10  | C24   | 1169 | ASN  | O-C-N  | -10.36 | 109.55      | 123.01   |
| 10  | C     | 1169 | ASN  | O-C-N  | -10.35 | 109.55      | 123.01   |
| 10  | C16   | 1169 | ASN  | O-C-N  | -10.35 | 109.56      | 123.01   |
| 2   | M     | 156  | GLY  | CA-C-N | 10.35  | 141.69      | 121.41   |
| 2   | M     | 156  | GLY  | C-N-CA | 10.35  | 141.69      | 121.41   |
| 18  | B     | 978  | ASN  | O-C-N  | -10.35 | 111.41      | 122.07   |
| 9   | K8    | 718  | PHE  | O-C-N  | -10.34 | 108.99      | 122.43   |
| 9   | K8    | 1193 | SER  | CA-C-N | 10.34  | 134.54      | 120.38   |
| 9   | K8    | 1193 | SER  | C-N-CA | 10.34  | 134.54      | 120.38   |
| 10  | C8    | 1169 | ASN  | O-C-N  | -10.33 | 109.58      | 123.01   |
| 14  | W     | 703  | GLY  | O-C-N  | -10.32 | 109.28      | 122.70   |
| 2   | M8    | 156  | GLY  | CA-C-N | 10.32  | 141.64      | 121.41   |
| 2   | M8    | 156  | GLY  | C-N-CA | 10.32  | 141.64      | 121.41   |
| 10  | C32   | 1169 | ASN  | O-C-N  | -10.31 | 109.61      | 123.01   |
| 1   | R8    | 1182 | PRO  | O-C-N  | -10.30 | 108.73      | 122.64   |
| 10  | C8    | 1167 | PHE  | O-C-N  | -10.30 | 109.47      | 121.32   |
| 18  | B8    | 993  | ALA  | O-C-N  | -10.30 | 108.89      | 122.59   |
| 18  | B8    | 681  | GLY  | CA-C-N | 10.30  | 134.92      | 120.29   |
| 18  | B8    | 681  | GLY  | C-N-CA | 10.30  | 134.92      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10  | C24   | 1540 | GLU  | O-C-N  | -10.29 | 109.84      | 122.71   |
| 10  | C16   | 1167 | PHE  | O-C-N  | -10.29 | 109.48      | 121.32   |
| 10  | C     | 1166 | SER  | O-C-N  | -10.29 | 109.12      | 122.39   |
| 10  | C32   | 627  | VAL  | O-C-N  | -10.29 | 109.71      | 122.57   |
| 12  | A48   | 241  | VAL  | O-C-N  | -10.29 | 109.71      | 122.57   |
| 18  | B     | 681  | GLY  | CA-C-N | 10.29  | 134.90      | 120.29   |
| 18  | B     | 681  | GLY  | C-N-CA | 10.29  | 134.90      | 120.29   |
| 1   | R     | 1182 | PRO  | O-C-N  | -10.28 | 108.76      | 122.64   |
| 10  | C16   | 1166 | SER  | O-C-N  | -10.28 | 109.12      | 122.39   |
| 10  | C8    | 1166 | SER  | O-C-N  | -10.27 | 109.14      | 122.39   |
| 1   | R16   | 1182 | PRO  | O-C-N  | -10.27 | 108.77      | 122.64   |
| 12  | A     | 467  | SER  | CA-C-N | -10.27 | 103.48      | 121.97   |
| 12  | A     | 467  | SER  | C-N-CA | -10.27 | 103.48      | 121.97   |
| 10  | C24   | 1166 | SER  | O-C-N  | -10.27 | 109.15      | 122.39   |
| 6   | O16   | 158  | ASP  | O-C-N  | -10.26 | 110.62      | 122.93   |
| 10  | C16   | 1540 | GLU  | O-C-N  | -10.26 | 109.89      | 122.71   |
| 10  | C32   | 1166 | SER  | O-C-N  | -10.26 | 109.16      | 122.39   |
| 18  | B     | 993  | ALA  | O-C-N  | -10.25 | 108.96      | 122.59   |
| 10  | C16   | 627  | VAL  | O-C-N  | -10.25 | 109.76      | 122.57   |
| 10  | C24   | 1167 | PHE  | O-C-N  | -10.25 | 109.54      | 121.32   |
| 10  | C32   | 1540 | GLU  | O-C-N  | -10.25 | 109.90      | 122.71   |
| 11  | A16   | 467  | SER  | CA-C-N | -10.24 | 103.54      | 121.97   |
| 11  | A16   | 467  | SER  | C-N-CA | -10.24 | 103.54      | 121.97   |
| 12  | A48   | 467  | SER  | CA-C-N | -10.24 | 103.54      | 121.97   |
| 12  | A48   | 467  | SER  | C-N-CA | -10.24 | 103.54      | 121.97   |
| 10  | C32   | 1167 | PHE  | O-C-N  | -10.24 | 109.55      | 121.32   |
| 9   | K8    | 1193 | SER  | O-C-N  | -10.23 | 110.78      | 122.75   |
| 10  | C24   | 627  | VAL  | O-C-N  | -10.23 | 109.79      | 122.57   |
| 10  | C     | 1167 | PHE  | O-C-N  | -10.23 | 109.56      | 121.32   |
| 11  | A32   | 467  | SER  | CA-C-N | -10.22 | 103.56      | 121.97   |
| 11  | A32   | 467  | SER  | C-N-CA | -10.22 | 103.56      | 121.97   |
| 11  | A40   | 467  | SER  | CA-C-N | -10.22 | 103.58      | 121.97   |
| 11  | A40   | 467  | SER  | C-N-CA | -10.22 | 103.58      | 121.97   |
| 11  | A24   | 467  | SER  | CA-C-N | -10.21 | 103.60      | 121.97   |
| 11  | A24   | 467  | SER  | C-N-CA | -10.21 | 103.60      | 121.97   |
| 6   | O8    | 158  | ASP  | O-C-N  | -10.20 | 110.69      | 122.93   |
| 6   | O     | 158  | ASP  | O-C-N  | -10.20 | 110.69      | 122.93   |
| 12  | A     | 241  | VAL  | O-C-N  | -10.20 | 109.82      | 122.57   |
| 10  | C     | 627  | VAL  | O-C-N  | -10.20 | 109.82      | 122.57   |
| 11  | A32   | 241  | VAL  | O-C-N  | -10.20 | 109.82      | 122.57   |
| 10  | C32   | 627  | VAL  | CA-C-N | 10.20  | 141.40      | 121.41   |
| 10  | C32   | 627  | VAL  | C-N-CA | 10.20  | 141.40      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 11  | A24   | 241  | VAL  | O-C-N  | -10.19 | 109.83      | 122.57   |
| 19  | 48    | 189  | LEU  | O-C-N  | -10.19 | 109.04      | 122.59   |
| 11  | A16   | 241  | VAL  | O-C-N  | -10.18 | 109.84      | 122.57   |
| 10  | C24   | 627  | VAL  | CA-C-N | 10.18  | 141.36      | 121.41   |
| 10  | C24   | 627  | VAL  | C-N-CA | 10.18  | 141.36      | 121.41   |
| 9   | K8    | 730  | SER  | O-C-N  | -10.17 | 111.72      | 123.11   |
| 10  | C16   | 622  | VAL  | O-C-N  | -10.16 | 109.87      | 122.57   |
| 19  | 4     | 189  | LEU  | O-C-N  | -10.16 | 109.08      | 122.59   |
| 10  | C16   | 627  | VAL  | CA-C-N | 10.16  | 141.32      | 121.41   |
| 10  | C16   | 627  | VAL  | C-N-CA | 10.16  | 141.32      | 121.41   |
| 18  | B8    | 1811 | PRO  | CA-C-N | 10.16  | 135.14      | 120.82   |
| 18  | B8    | 1811 | PRO  | C-N-CA | 10.16  | 135.14      | 120.82   |
| 18  | B     | 1811 | PRO  | CA-C-N | 10.15  | 135.14      | 120.82   |
| 18  | B     | 1811 | PRO  | C-N-CA | 10.15  | 135.14      | 120.82   |
| 9   | K     | 1059 | ARG  | O-C-N  | -10.14 | 109.10      | 122.59   |
| 11  | A40   | 241  | VAL  | O-C-N  | -10.14 | 109.89      | 122.57   |
| 9   | K     | 730  | SER  | O-C-N  | -10.14 | 111.75      | 123.11   |
| 10  | C32   | 622  | VAL  | O-C-N  | -10.13 | 109.90      | 122.57   |
| 9   | K     | 1276 | VAL  | CA-C-N | 10.13  | 140.89      | 121.54   |
| 9   | K     | 1276 | VAL  | C-N-CA | 10.13  | 140.89      | 121.54   |
| 10  | C     | 627  | VAL  | CA-C-N | 10.13  | 141.26      | 121.41   |
| 10  | C     | 627  | VAL  | C-N-CA | 10.13  | 141.26      | 121.41   |
| 10  | C32   | 1625 | SER  | O-C-N  | -10.12 | 110.33      | 122.89   |
| 9   | K8    | 1059 | ARG  | O-C-N  | -10.12 | 109.13      | 122.59   |
| 10  | C24   | 1625 | SER  | O-C-N  | -10.12 | 110.34      | 122.89   |
| 10  | C8    | 1625 | SER  | O-C-N  | -10.11 | 110.35      | 122.89   |
| 9   | K8    | 1276 | VAL  | CA-C-N | 10.11  | 140.85      | 121.54   |
| 9   | K8    | 1276 | VAL  | C-N-CA | 10.11  | 140.85      | 121.54   |
| 10  | C     | 1625 | SER  | O-C-N  | -10.10 | 110.37      | 122.89   |
| 1   | R16   | 1192 | LYS  | O-C-N  | -10.10 | 109.16      | 122.59   |
| 7   | Q8    | 222  | PHE  | O-C-N  | -10.08 | 108.37      | 121.97   |
| 10  | C     | 622  | VAL  | O-C-N  | -10.08 | 109.97      | 122.57   |
| 10  | C16   | 1625 | SER  | O-C-N  | -10.07 | 110.41      | 122.89   |
| 18  | B     | 1478 | MET  | CA-C-N | 10.07  | 141.14      | 121.41   |
| 18  | B     | 1478 | MET  | C-N-CA | 10.07  | 141.14      | 121.41   |
| 7   | Q     | 222  | PHE  | O-C-N  | -10.06 | 108.38      | 121.97   |
| 10  | C16   | 1660 | SER  | O-C-N  | -10.06 | 108.20      | 122.29   |
| 18  | B8    | 124  | THR  | O-C-N  | -10.06 | 110.56      | 122.93   |
| 2   | M16   | 347  | LYS  | O-C-N  | -10.05 | 109.22      | 122.59   |
| 18  | B     | 124  | THR  | O-C-N  | -10.05 | 110.57      | 122.93   |
| 2   | M8    | 347  | LYS  | O-C-N  | -10.04 | 109.23      | 122.59   |
| 10  | C24   | 622  | VAL  | O-C-N  | -10.05 | 110.01      | 122.57   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 7   | Q16   | 222  | PHE  | O-C-N  | -10.04 | 108.41      | 121.97   |
| 10  | C8    | 282  | LYS  | O-C-N  | -10.04 | 110.67      | 123.02   |
| 19  | 48    | 374  | GLY  | O-C-N  | 10.04  | 133.53      | 123.48   |
| 1   | R     | 1192 | LYS  | O-C-N  | -10.04 | 109.24      | 122.59   |
| 18  | B8    | 1133 | THR  | O-C-N  | -10.04 | 110.44      | 122.89   |
| 18  | B8    | 1478 | MET  | CA-C-N | 10.04  | 141.08      | 121.41   |
| 18  | B8    | 1478 | MET  | C-N-CA | 10.04  | 141.08      | 121.41   |
| 10  | C24   | 282  | LYS  | O-C-N  | -10.03 | 110.69      | 123.02   |
| 1   | R8    | 1192 | LYS  | O-C-N  | -10.03 | 109.25      | 122.59   |
| 18  | B     | 1133 | THR  | O-C-N  | -10.03 | 110.46      | 122.89   |
| 20  | E8    | 429  | PRO  | CA-C-N | 10.03  | 144.98      | 121.52   |
| 20  | E8    | 429  | PRO  | C-N-CA | 10.03  | 144.98      | 121.52   |
| 10  | C     | 282  | LYS  | O-C-N  | -10.02 | 110.69      | 123.02   |
| 10  | C     | 1660 | SER  | O-C-N  | -10.02 | 108.26      | 122.29   |
| 10  | C32   | 1660 | SER  | O-C-N  | -10.02 | 108.27      | 122.29   |
| 10  | C16   | 282  | LYS  | O-C-N  | -10.01 | 110.70      | 123.02   |
| 7   | Q8    | 298  | SER  | O-C-N  | -10.01 | 110.48      | 122.89   |
| 2   | M     | 347  | LYS  | O-C-N  | -10.01 | 109.28      | 122.59   |
| 5   | P8    | 592  | SER  | O-C-N  | -10.01 | 109.16      | 122.57   |
| 18  | B8    | 985  | ASP  | O-C-N  | -10.00 | 107.58      | 122.28   |
| 20  | E     | 429  | PRO  | CA-C-N | 10.00  | 144.92      | 121.52   |
| 20  | E     | 429  | PRO  | C-N-CA | 10.00  | 144.92      | 121.52   |
| 19  | 4     | 374  | GLY  | O-C-N  | 10.00  | 133.48      | 123.48   |
| 10  | C32   | 282  | LYS  | O-C-N  | -10.00 | 110.72      | 123.02   |
| 1   | R16   | 1144 | CYS  | O-C-N  | -9.99  | 108.81      | 122.20   |
| 1   | R     | 1144 | CYS  | O-C-N  | -9.99  | 108.82      | 122.20   |
| 18  | B8    | 114  | GLY  | O-C-N  | -9.98  | 109.73      | 122.70   |
| 5   | P16   | 592  | SER  | O-C-N  | -9.97  | 109.21      | 122.57   |
| 7   | Q16   | 298  | SER  | O-C-N  | -9.96  | 110.54      | 122.89   |
| 1   | R8    | 1144 | CYS  | O-C-N  | -9.96  | 108.86      | 122.20   |
| 9   | K8    | 1275 | ILE  | CA-C-N | 9.96   | 139.89      | 121.97   |
| 9   | K8    | 1275 | ILE  | C-N-CA | 9.96   | 139.89      | 121.97   |
| 5   | P     | 592  | SER  | O-C-N  | -9.96  | 109.23      | 122.57   |
| 9   | K     | 1275 | ILE  | CA-C-N | 9.95   | 139.88      | 121.97   |
| 9   | K     | 1275 | ILE  | C-N-CA | 9.95   | 139.88      | 121.97   |
| 10  | C24   | 1660 | SER  | O-C-N  | -9.95  | 108.36      | 122.29   |
| 18  | B     | 985  | ASP  | O-C-N  | -9.94  | 107.67      | 122.28   |
| 18  | B     | 114  | GLY  | O-C-N  | -9.92  | 109.81      | 122.70   |
| 7   | Q     | 298  | SER  | O-C-N  | -9.92  | 110.59      | 122.89   |
| 9   | K8    | 857  | ASP  | O-C-N  | -9.91  | 111.17      | 123.06   |
| 20  | E8    | 343  | THR  | CA-C-N | 9.91   | 132.22      | 119.84   |
| 20  | E8    | 343  | THR  | C-N-CA | 9.91   | 132.22      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 449  | GLU  | CA-C-N | 9.90  | 129.27      | 118.97   |
| 10  | C16   | 449  | GLU  | C-N-CA | 9.90  | 129.27      | 118.97   |
| 18  | B     | 1804 | THR  | CA-C-N | -9.90 | 106.66      | 120.71   |
| 18  | B     | 1804 | THR  | C-N-CA | -9.90 | 106.66      | 120.71   |
| 17  | F16   | 74   | ILE  | O-C-N  | -9.89 | 110.20      | 122.57   |
| 20  | E     | 343  | THR  | CA-C-N | 9.89  | 132.20      | 119.84   |
| 20  | E     | 343  | THR  | C-N-CA | 9.89  | 132.20      | 119.84   |
| 10  | C32   | 449  | GLU  | CA-C-N | 9.88  | 129.25      | 118.97   |
| 10  | C32   | 449  | GLU  | C-N-CA | 9.88  | 129.25      | 118.97   |
| 10  | C16   | 1353 | ASP  | O-C-N  | -9.88 | 109.45      | 122.59   |
| 2   | M8    | 345  | ASP  | CA-C-N | -9.88 | 104.19      | 121.97   |
| 2   | M8    | 345  | ASP  | C-N-CA | -9.88 | 104.19      | 121.97   |
| 2   | M16   | 345  | ASP  | CA-C-N | -9.88 | 104.19      | 121.97   |
| 2   | M16   | 345  | ASP  | C-N-CA | -9.88 | 104.19      | 121.97   |
| 9   | K     | 857  | ASP  | O-C-N  | -9.87 | 111.22      | 123.06   |
| 18  | B8    | 1804 | THR  | CA-C-N | -9.87 | 106.70      | 120.71   |
| 18  | B8    | 1804 | THR  | C-N-CA | -9.87 | 106.70      | 120.71   |
| 10  | C24   | 449  | GLU  | CA-C-N | 9.86  | 129.23      | 118.97   |
| 10  | C24   | 449  | GLU  | C-N-CA | 9.86  | 129.23      | 118.97   |
| 10  | C24   | 1353 | ASP  | O-C-N  | -9.86 | 109.48      | 122.59   |
| 17  | F24   | 74   | ILE  | O-C-N  | -9.85 | 110.26      | 122.57   |
| 10  | C     | 1353 | ASP  | O-C-N  | -9.84 | 109.51      | 122.59   |
| 5   | P16   | 391  | LYS  | O-C-N  | 9.84  | 130.31      | 121.36   |
| 18  | B8    | 606  | GLN  | O-C-N  | -9.84 | 109.67      | 122.56   |
| 2   | M     | 345  | ASP  | CA-C-N | -9.83 | 104.28      | 121.97   |
| 2   | M     | 345  | ASP  | C-N-CA | -9.83 | 104.28      | 121.97   |
| 10  | C32   | 1353 | ASP  | O-C-N  | -9.82 | 109.52      | 122.59   |
| 5   | P8    | 16   | PHE  | CA-C-N | -9.82 | 106.26      | 122.17   |
| 5   | P8    | 16   | PHE  | C-N-CA | -9.82 | 106.26      | 122.17   |
| 9   | K     | 723  | ALA  | CA-C-N | 9.82  | 140.66      | 121.41   |
| 9   | K     | 723  | ALA  | C-N-CA | 9.82  | 140.66      | 121.41   |
| 18  | B     | 606  | GLN  | O-C-N  | -9.82 | 109.70      | 122.56   |
| 17  | F     | 74   | ILE  | O-C-N  | -9.82 | 110.30      | 122.57   |
| 14  | W     | 584  | CYS  | CA-C-N | 9.81  | 139.64      | 121.97   |
| 14  | W     | 584  | CYS  | C-N-CA | 9.81  | 139.64      | 121.97   |
| 9   | K8    | 723  | ALA  | CA-C-N | 9.81  | 140.64      | 121.41   |
| 9   | K8    | 723  | ALA  | C-N-CA | 9.81  | 140.64      | 121.41   |
| 10  | C8    | 1066 | SER  | O-C-N  | -9.81 | 109.54      | 122.59   |
| 5   | P     | 16   | PHE  | CA-C-N | -9.81 | 106.28      | 122.17   |
| 5   | P     | 16   | PHE  | C-N-CA | -9.81 | 106.28      | 122.17   |
| 17  | F8    | 74   | ILE  | O-C-N  | -9.80 | 110.31      | 122.57   |
| 10  | C8    | 1110 | SER  | CA-C-N | -9.80 | 106.37      | 121.66   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1110 | SER  | C-N-CA | -9.80 | 106.37      | 121.66   |
| 18  | B     | 614  | MET  | O-C-N  | -9.80 | 109.56      | 122.59   |
| 10  | C     | 1110 | SER  | CA-C-N | -9.79 | 106.39      | 121.66   |
| 10  | C     | 1110 | SER  | C-N-CA | -9.79 | 106.39      | 121.66   |
| 18  | B8    | 682  | TYR  | O-C-N  | -9.79 | 110.99      | 122.15   |
| 10  | C32   | 1066 | SER  | O-C-N  | -9.78 | 109.58      | 122.59   |
| 10  | C8    | 1353 | ASP  | O-C-N  | -9.78 | 109.59      | 122.59   |
| 5   | P16   | 16   | PHE  | CA-C-N | -9.77 | 106.34      | 122.17   |
| 5   | P16   | 16   | PHE  | C-N-CA | -9.77 | 106.34      | 122.17   |
| 18  | B     | 1803 | THR  | O-C-N  | -9.77 | 109.59      | 122.59   |
| 18  | B8    | 1803 | THR  | O-C-N  | -9.77 | 109.59      | 122.59   |
| 10  | C16   | 1110 | SER  | CA-C-N | -9.77 | 106.42      | 121.66   |
| 10  | C16   | 1110 | SER  | C-N-CA | -9.77 | 106.42      | 121.66   |
| 10  | C32   | 1110 | SER  | CA-C-N | -9.77 | 106.42      | 121.66   |
| 10  | C32   | 1110 | SER  | C-N-CA | -9.77 | 106.42      | 121.66   |
| 6   | O     | 160  | LEU  | CA-C-N | -9.77 | 108.05      | 122.41   |
| 6   | O     | 160  | LEU  | C-N-CA | -9.77 | 108.05      | 122.41   |
| 10  | C     | 1066 | SER  | O-C-N  | -9.77 | 109.60      | 122.59   |
| 5   | P8    | 391  | LYS  | O-C-N  | 9.76  | 130.24      | 121.36   |
| 6   | O8    | 160  | LEU  | CA-C-N | -9.76 | 108.06      | 122.41   |
| 6   | O8    | 160  | LEU  | C-N-CA | -9.76 | 108.06      | 122.41   |
| 5   | P     | 391  | LYS  | O-C-N  | 9.75  | 130.23      | 121.36   |
| 18  | B8    | 614  | MET  | O-C-N  | -9.75 | 109.62      | 122.59   |
| 10  | C16   | 1066 | SER  | O-C-N  | -9.74 | 109.63      | 122.59   |
| 10  | C24   | 1066 | SER  | O-C-N  | -9.74 | 109.64      | 122.59   |
| 5   | P     | 657  | TRP  | O-C-N  | -9.74 | 112.84      | 121.31   |
| 10  | C24   | 1351 | GLU  | O-C-N  | -9.74 | 111.51      | 122.03   |
| 18  | B     | 682  | TYR  | O-C-N  | -9.74 | 111.05      | 122.15   |
| 6   | O16   | 160  | LEU  | CA-C-N | -9.73 | 108.10      | 122.41   |
| 6   | O16   | 160  | LEU  | C-N-CA | -9.73 | 108.10      | 122.41   |
| 6   | O8    | 94   | GLY  | CA-C-N | 9.72  | 135.40      | 121.02   |
| 6   | O8    | 94   | GLY  | C-N-CA | 9.72  | 135.40      | 121.02   |
| 6   | O16   | 94   | GLY  | CA-C-N | 9.72  | 135.40      | 121.02   |
| 6   | O16   | 94   | GLY  | C-N-CA | 9.72  | 135.40      | 121.02   |
| 7   | Q16   | 219  | GLY  | O-C-N  | -9.71 | 110.08      | 122.70   |
| 13  | V     | 883  | PRO  | CA-C-N | -9.71 | 105.82      | 121.26   |
| 13  | V     | 883  | PRO  | C-N-CA | -9.71 | 105.82      | 121.26   |
| 6   | O8    | 93   | HIS  | O-C-N  | -9.70 | 111.84      | 123.29   |
| 10  | C16   | 1351 | GLU  | O-C-N  | -9.70 | 111.55      | 122.03   |
| 10  | C24   | 1110 | SER  | CA-C-N | -9.70 | 106.53      | 121.66   |
| 10  | C24   | 1110 | SER  | C-N-CA | -9.70 | 106.53      | 121.66   |
| 19  | 4     | 70   | SER  | CA-C-N | -9.70 | 103.02      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 19  | 4     | 70   | SER  | C-N-CA     | -9.70 | 103.02      | 121.54   |
| 6   | O     | 94   | GLY  | CA-C-N     | 9.69  | 135.36      | 121.02   |
| 6   | O     | 94   | GLY  | C-N-CA     | 9.69  | 135.36      | 121.02   |
| 1   | R16   | 529  | HIS  | CG-ND1-CE1 | 9.69  | 125.77      | 109.30   |
| 19  | 48    | 70   | SER  | CA-C-N     | -9.69 | 103.04      | 121.54   |
| 19  | 48    | 70   | SER  | C-N-CA     | -9.69 | 103.04      | 121.54   |
| 1   | R8    | 529  | HIS  | CG-ND1-CE1 | 9.68  | 125.76      | 109.30   |
| 10  | C8    | 1351 | GLU  | O-C-N      | -9.68 | 111.58      | 122.03   |
| 7   | Q     | 219  | GLY  | O-C-N      | -9.68 | 110.12      | 122.70   |
| 13  | V     | 881  | GLY  | O-C-N      | -9.68 | 110.12      | 122.70   |
| 6   | O     | 93   | HIS  | O-C-N      | -9.67 | 111.88      | 123.29   |
| 10  | C16   | 1276 | SER  | CA-C-N     | -9.67 | 110.27      | 122.84   |
| 10  | C16   | 1276 | SER  | C-N-CA     | -9.67 | 110.27      | 122.84   |
| 6   | O16   | 93   | HIS  | O-C-N      | -9.67 | 111.88      | 123.29   |
| 10  | C24   | 1276 | SER  | CA-C-N     | -9.67 | 110.27      | 122.84   |
| 10  | C24   | 1276 | SER  | C-N-CA     | -9.67 | 110.27      | 122.84   |
| 7   | Q8    | 219  | GLY  | O-C-N      | -9.66 | 110.14      | 122.70   |
| 10  | C32   | 1351 | GLU  | O-C-N      | -9.66 | 111.59      | 122.03   |
| 5   | P8    | 207  | HIS  | O-C-N      | 9.65  | 128.70      | 121.65   |
| 18  | B     | 1278 | LYS  | O-C-N      | -9.65 | 108.78      | 122.29   |
| 1   | R     | 529  | HIS  | CG-ND1-CE1 | 9.64  | 125.69      | 109.30   |
| 10  | C32   | 1276 | SER  | CA-C-N     | -9.64 | 110.31      | 122.84   |
| 10  | C32   | 1276 | SER  | C-N-CA     | -9.64 | 110.31      | 122.84   |
| 18  | B8    | 1278 | LYS  | O-C-N      | -9.63 | 108.81      | 122.29   |
| 5   | P8    | 657  | TRP  | O-C-N      | -9.62 | 112.94      | 121.31   |
| 10  | C     | 1351 | GLU  | O-C-N      | -9.62 | 111.64      | 122.03   |
| 10  | C8    | 1276 | SER  | CA-C-N     | -9.62 | 110.34      | 122.84   |
| 10  | C8    | 1276 | SER  | C-N-CA     | -9.62 | 110.34      | 122.84   |
| 5   | P     | 207  | HIS  | O-C-N      | 9.61  | 128.67      | 121.65   |
| 10  | C     | 1276 | SER  | CA-C-N     | -9.60 | 110.36      | 122.84   |
| 10  | C     | 1276 | SER  | C-N-CA     | -9.60 | 110.36      | 122.84   |
| 10  | C     | 1785 | SER  | CA-C-N     | 9.59  | 134.09      | 120.28   |
| 10  | C     | 1785 | SER  | C-N-CA     | 9.59  | 134.09      | 120.28   |
| 18  | B     | 2    | ALA  | O-C-N      | -9.59 | 109.84      | 122.59   |
| 10  | C16   | 1785 | SER  | CA-C-N     | 9.58  | 134.08      | 120.28   |
| 10  | C16   | 1785 | SER  | C-N-CA     | 9.58  | 134.08      | 120.28   |
| 20  | E8    | 427  | MET  | O-C-N      | -9.57 | 109.25      | 122.46   |
| 10  | C     | 1777 | SER  | CA-C-N     | -9.57 | 108.02      | 120.65   |
| 10  | C     | 1777 | SER  | C-N-CA     | -9.57 | 108.02      | 120.65   |
| 10  | C8    | 1777 | SER  | CA-C-N     | -9.57 | 108.02      | 120.65   |
| 10  | C8    | 1777 | SER  | C-N-CA     | -9.57 | 108.02      | 120.65   |
| 10  | C     | 334  | MET  | O-C-N      | -9.56 | 110.54      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | P16   | 207  | HIS  | O-C-N      | 9.56  | 128.63      | 121.65   |
| 18  | B8    | 2    | ALA  | O-C-N      | -9.55 | 109.88      | 122.59   |
| 10  | C16   | 334  | MET  | O-C-N      | -9.55 | 110.55      | 122.68   |
| 10  | C32   | 334  | MET  | O-C-N      | -9.55 | 110.56      | 122.68   |
| 18  | B8    | 693  | SER  | O-C-N      | -9.54 | 111.61      | 123.06   |
| 10  | C24   | 1777 | SER  | CA-C-N     | -9.54 | 108.06      | 120.65   |
| 10  | C24   | 1777 | SER  | C-N-CA     | -9.54 | 108.06      | 120.65   |
| 18  | B     | 693  | SER  | O-C-N      | -9.54 | 111.61      | 123.06   |
| 18  | B     | 991  | ASP  | O-C-N      | -9.54 | 109.90      | 122.59   |
| 10  | C24   | 1785 | SER  | CA-C-N     | 9.54  | 134.01      | 120.28   |
| 10  | C24   | 1785 | SER  | C-N-CA     | 9.54  | 134.01      | 120.28   |
| 14  | W     | 587  | SER  | O-C-N      | -9.54 | 111.20      | 122.93   |
| 20  | E     | 427  | MET  | O-C-N      | -9.54 | 109.30      | 122.46   |
| 8   | L16   | 1054 | HIS  | CG-ND1-CE1 | 9.53  | 125.50      | 109.30   |
| 12  | A     | 552  | GLY  | O-C-N      | -9.53 | 110.31      | 122.70   |
| 10  | C24   | 334  | MET  | O-C-N      | -9.53 | 110.58      | 122.68   |
| 18  | B8    | 991  | ASP  | O-C-N      | -9.53 | 109.91      | 122.59   |
| 10  | C32   | 1785 | SER  | CA-C-N     | 9.53  | 134.01      | 120.28   |
| 10  | C32   | 1785 | SER  | C-N-CA     | 9.53  | 134.01      | 120.28   |
| 5   | P16   | 657  | TRP  | O-C-N      | -9.53 | 113.02      | 121.31   |
| 10  | C16   | 1777 | SER  | CA-C-N     | -9.53 | 108.07      | 120.65   |
| 10  | C16   | 1777 | SER  | C-N-CA     | -9.53 | 108.07      | 120.65   |
| 10  | C24   | 629  | LYS  | O-C-N      | -9.53 | 109.92      | 122.59   |
| 9   | K     | 1064 | PRO  | O-C-N      | -9.52 | 109.78      | 122.64   |
| 9   | K8    | 1064 | PRO  | O-C-N      | -9.52 | 109.79      | 122.64   |
| 10  | C8    | 1068 | THR  | CA-C-N     | -9.52 | 107.91      | 120.67   |
| 10  | C8    | 1068 | THR  | C-N-CA     | -9.52 | 107.91      | 120.67   |
| 18  | B8    | 1068 | THR  | O-C-N      | -9.52 | 109.93      | 122.59   |
| 10  | C8    | 1498 | GLY  | O-C-N      | -9.52 | 115.00      | 123.37   |
| 10  | C8    | 1785 | SER  | CA-C-N     | 9.52  | 133.98      | 120.28   |
| 10  | C8    | 1785 | SER  | C-N-CA     | 9.52  | 133.98      | 120.28   |
| 10  | C16   | 629  | LYS  | O-C-N      | -9.51 | 109.94      | 122.59   |
| 10  | C     | 428  | GLY  | O-C-N      | -9.51 | 110.33      | 122.70   |
| 8   | L     | 1054 | HIS  | CG-ND1-CE1 | 9.51  | 125.47      | 109.30   |
| 18  | B     | 1068 | THR  | O-C-N      | -9.51 | 109.94      | 122.59   |
| 9   | K8    | 892  | GLU  | O-C-N      | -9.51 | 109.95      | 122.59   |
| 10  | C24   | 1068 | THR  | CA-C-N     | -9.51 | 107.93      | 120.67   |
| 10  | C24   | 1068 | THR  | C-N-CA     | -9.51 | 107.93      | 120.67   |
| 10  | C16   | 428  | GLY  | O-C-N      | -9.50 | 110.35      | 122.70   |
| 8   | L8    | 1054 | HIS  | CG-ND1-CE1 | 9.50  | 125.45      | 109.30   |
| 10  | C     | 629  | LYS  | O-C-N      | -9.50 | 109.95      | 122.59   |
| 10  | C32   | 629  | LYS  | O-C-N      | -9.50 | 109.95      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 428  | GLY  | O-C-N  | -9.49 | 110.36      | 122.70   |
| 9   | K     | 857  | ASP  | CA-C-N | 9.49  | 136.18      | 120.62   |
| 9   | K     | 857  | ASP  | C-N-CA | 9.49  | 136.18      | 120.62   |
| 18  | B8    | 116  | THR  | CA-C-N | 9.48  | 139.66      | 121.54   |
| 18  | B8    | 116  | THR  | C-N-CA | 9.48  | 139.66      | 121.54   |
| 10  | C8    | 334  | MET  | O-C-N  | -9.48 | 110.64      | 122.68   |
| 18  | B     | 116  | THR  | CA-C-N | 9.48  | 139.64      | 121.54   |
| 18  | B     | 116  | THR  | C-N-CA | 9.48  | 139.64      | 121.54   |
| 9   | K8    | 640  | THR  | O-C-N  | -9.47 | 112.08      | 122.12   |
| 9   | K8    | 857  | ASP  | CA-C-N | 9.47  | 136.15      | 120.62   |
| 9   | K8    | 857  | ASP  | C-N-CA | 9.47  | 136.15      | 120.62   |
| 10  | C32   | 1777 | SER  | CA-C-N | -9.47 | 108.15      | 120.65   |
| 10  | C32   | 1777 | SER  | C-N-CA | -9.47 | 108.15      | 120.65   |
| 10  | C16   | 1498 | GLY  | O-C-N  | -9.47 | 115.04      | 123.37   |
| 12  | A48   | 552  | GLY  | O-C-N  | -9.47 | 110.39      | 122.70   |
| 10  | C8    | 428  | GLY  | O-C-N  | -9.47 | 110.39      | 122.70   |
| 9   | K8    | 643  | GLY  | O-C-N  | -9.46 | 111.97      | 122.28   |
| 11  | A40   | 552  | GLY  | O-C-N  | -9.46 | 110.40      | 122.70   |
| 10  | C     | 1068 | THR  | CA-C-N | -9.46 | 107.99      | 120.67   |
| 10  | C     | 1068 | THR  | C-N-CA | -9.46 | 107.99      | 120.67   |
| 10  | C32   | 1068 | THR  | CA-C-N | -9.46 | 107.99      | 120.67   |
| 10  | C32   | 1068 | THR  | C-N-CA | -9.46 | 107.99      | 120.67   |
| 10  | C24   | 508  | ILE  | O-C-N  | -9.46 | 113.17      | 123.20   |
| 11  | A32   | 552  | GLY  | O-C-N  | -9.45 | 110.42      | 122.70   |
| 18  | B     | 500  | THR  | O-C-N  | -9.45 | 112.24      | 123.10   |
| 10  | C32   | 1498 | GLY  | O-C-N  | -9.45 | 115.06      | 123.37   |
| 10  | C24   | 428  | GLY  | O-C-N  | -9.44 | 110.43      | 122.70   |
| 10  | C     | 508  | ILE  | O-C-N  | -9.44 | 113.19      | 123.20   |
| 10  | C     | 1498 | GLY  | O-C-N  | -9.44 | 115.06      | 123.37   |
| 9   | K     | 640  | THR  | O-C-N  | -9.44 | 112.12      | 122.12   |
| 9   | K     | 892  | GLU  | O-C-N  | -9.44 | 110.04      | 122.59   |
| 10  | C16   | 1068 | THR  | CA-C-N | -9.44 | 108.03      | 120.67   |
| 10  | C16   | 1068 | THR  | C-N-CA | -9.44 | 108.03      | 120.67   |
| 10  | C24   | 1067 | SER  | O-C-N  | -9.43 | 110.05      | 122.59   |
| 10  | C     | 1067 | SER  | O-C-N  | -9.43 | 110.05      | 122.59   |
| 11  | A16   | 552  | GLY  | O-C-N  | -9.43 | 110.45      | 122.70   |
| 19  | 48    | 188  | ALA  | O-C-N  | -9.42 | 110.07      | 122.59   |
| 9   | K     | 643  | GLY  | O-C-N  | -9.41 | 112.02      | 122.28   |
| 9   | K8    | 926  | ILE  | O-C-N  | -9.41 | 112.42      | 122.68   |
| 11  | A24   | 552  | GLY  | O-C-N  | -9.41 | 110.46      | 122.70   |
| 10  | C16   | 508  | ILE  | O-C-N  | -9.41 | 113.22      | 123.20   |
| 10  | C     | 1497 | LYS  | O-C-N  | -9.41 | 110.32      | 122.37   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 19  | 4     | 188  | ALA  | O-C-N  | -9.40 | 110.08      | 122.59   |
| 10  | C24   | 1442 | GLN  | CA-C-N | -9.40 | 107.75      | 122.23   |
| 10  | C24   | 1442 | GLN  | C-N-CA | -9.40 | 107.75      | 122.23   |
| 10  | C8    | 1067 | SER  | O-C-N  | -9.40 | 110.08      | 122.59   |
| 9   | K     | 926  | ILE  | O-C-N  | -9.40 | 112.43      | 122.68   |
| 7   | Q8    | 57   | ASN  | CA-C-N | -9.40 | 109.68      | 119.83   |
| 7   | Q8    | 57   | ASN  | C-N-CA | -9.40 | 109.68      | 119.83   |
| 10  | C32   | 1062 | GLU  | CA-C-N | 9.39  | 131.58      | 119.84   |
| 10  | C32   | 1062 | GLU  | C-N-CA | 9.39  | 131.58      | 119.84   |
| 10  | C24   | 1498 | GLY  | O-C-N  | -9.39 | 115.10      | 123.37   |
| 10  | C32   | 1497 | LYS  | O-C-N  | -9.39 | 110.35      | 122.37   |
| 10  | C16   | 1497 | LYS  | O-C-N  | -9.39 | 110.35      | 122.37   |
| 7   | Q     | 57   | ASN  | CA-C-N | -9.39 | 109.69      | 119.83   |
| 7   | Q     | 57   | ASN  | C-N-CA | -9.39 | 109.69      | 119.83   |
| 18  | B8    | 500  | THR  | O-C-N  | -9.39 | 112.31      | 123.10   |
| 23  | J24   | 731  | LEU  | O-C-N  | 9.38  | 132.85      | 122.15   |
| 12  | A     | 268  | GLN  | O-C-N  | -9.38 | 110.63      | 122.82   |
| 11  | A32   | 268  | GLN  | O-C-N  | -9.38 | 110.63      | 122.82   |
| 10  | C32   | 1067 | SER  | O-C-N  | -9.38 | 110.12      | 122.59   |
| 10  | C     | 1062 | GLU  | CA-C-N | 9.37  | 131.56      | 119.84   |
| 10  | C     | 1062 | GLU  | C-N-CA | 9.37  | 131.56      | 119.84   |
| 23  | J16   | 731  | LEU  | O-C-N  | 9.37  | 132.84      | 122.15   |
| 12  | A48   | 268  | GLN  | O-C-N  | -9.37 | 110.64      | 122.82   |
| 10  | C8    | 1062 | GLU  | CA-C-N | 9.37  | 131.55      | 119.84   |
| 10  | C8    | 1062 | GLU  | C-N-CA | 9.37  | 131.55      | 119.84   |
| 11  | A40   | 268  | GLN  | O-C-N  | -9.36 | 110.65      | 122.82   |
| 7   | Q16   | 57   | ASN  | CA-C-N | -9.36 | 109.73      | 119.83   |
| 7   | Q16   | 57   | ASN  | C-N-CA | -9.36 | 109.73      | 119.83   |
| 14  | W     | 594  | PRO  | O-C-N  | -9.36 | 112.62      | 123.10   |
| 10  | C24   | 1062 | GLU  | CA-C-N | 9.35  | 131.53      | 119.84   |
| 10  | C24   | 1062 | GLU  | C-N-CA | 9.35  | 131.53      | 119.84   |
| 10  | C24   | 1497 | LYS  | O-C-N  | -9.35 | 110.40      | 122.37   |
| 11  | A16   | 27   | SER  | CA-C-N | -9.35 | 109.67      | 122.30   |
| 11  | A16   | 27   | SER  | C-N-CA | -9.35 | 109.67      | 122.30   |
| 10  | C16   | 1062 | GLU  | CA-C-N | 9.35  | 131.53      | 119.84   |
| 10  | C16   | 1062 | GLU  | C-N-CA | 9.35  | 131.53      | 119.84   |
| 10  | C     | 1442 | GLN  | CA-C-N | -9.35 | 107.83      | 122.23   |
| 10  | C     | 1442 | GLN  | C-N-CA | -9.35 | 107.83      | 122.23   |
| 11  | A24   | 268  | GLN  | O-C-N  | -9.35 | 110.67      | 122.82   |
| 23  | J32   | 731  | LEU  | O-C-N  | 9.35  | 132.80      | 122.15   |
| 11  | A32   | 27   | SER  | CA-C-N | -9.34 | 109.69      | 122.30   |
| 11  | A32   | 27   | SER  | C-N-CA | -9.34 | 109.69      | 122.30   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1497 | LYS  | O-C-N  | -9.34 | 110.42      | 122.37   |
| 11  | A40   | 27   | SER  | CA-C-N | -9.33 | 109.70      | 122.30   |
| 11  | A40   | 27   | SER  | C-N-CA | -9.33 | 109.70      | 122.30   |
| 11  | A24   | 27   | SER  | CA-C-N | -9.33 | 109.70      | 122.30   |
| 11  | A24   | 27   | SER  | C-N-CA | -9.33 | 109.70      | 122.30   |
| 10  | C16   | 1442 | GLN  | CA-C-N | -9.33 | 107.87      | 122.23   |
| 10  | C16   | 1442 | GLN  | C-N-CA | -9.33 | 107.87      | 122.23   |
| 23  | J8    | 731  | LEU  | O-C-N  | 9.33  | 132.78      | 122.15   |
| 10  | C32   | 508  | ILE  | O-C-N  | -9.32 | 113.33      | 123.20   |
| 10  | C32   | 1442 | GLN  | CA-C-N | -9.32 | 107.88      | 122.23   |
| 10  | C32   | 1442 | GLN  | C-N-CA | -9.32 | 107.88      | 122.23   |
| 10  | C16   | 1057 | THR  | CA-C-N | 9.31  | 139.33      | 121.54   |
| 10  | C16   | 1057 | THR  | C-N-CA | 9.31  | 139.33      | 121.54   |
| 10  | C8    | 1442 | GLN  | CA-C-N | -9.31 | 107.89      | 122.23   |
| 10  | C8    | 1442 | GLN  | C-N-CA | -9.31 | 107.89      | 122.23   |
| 20  | E8    | 352  | PHE  | O-C-N  | -9.31 | 110.20      | 122.59   |
| 11  | A16   | 268  | GLN  | O-C-N  | -9.31 | 110.72      | 122.82   |
| 18  | B8    | 1116 | GLU  | CA-C-N | -9.31 | 103.76      | 121.54   |
| 18  | B8    | 1116 | GLU  | C-N-CA | -9.31 | 103.76      | 121.54   |
| 10  | C8    | 1057 | THR  | CA-C-N | 9.30  | 139.30      | 121.54   |
| 10  | C8    | 1057 | THR  | C-N-CA | 9.30  | 139.30      | 121.54   |
| 18  | B8    | 1362 | ALA  | O-C-N  | -9.30 | 111.58      | 123.02   |
| 10  | C16   | 1067 | SER  | O-C-N  | -9.29 | 110.23      | 122.59   |
| 18  | B     | 1116 | GLU  | CA-C-N | -9.29 | 103.79      | 121.54   |
| 18  | B     | 1116 | GLU  | C-N-CA | -9.29 | 103.79      | 121.54   |
| 18  | B8    | 1962 | PRO  | O-C-N  | -9.29 | 112.32      | 123.01   |
| 18  | B     | 1362 | ALA  | O-C-N  | -9.29 | 111.59      | 123.02   |
| 10  | C32   | 1057 | THR  | CA-C-N | 9.28  | 139.27      | 121.54   |
| 10  | C32   | 1057 | THR  | C-N-CA | 9.28  | 139.27      | 121.54   |
| 20  | E     | 352  | PHE  | O-C-N  | -9.28 | 110.25      | 122.59   |
| 10  | C32   | 1223 | ASP  | O-C-N  | -9.26 | 112.49      | 122.96   |
| 10  | C24   | 1057 | THR  | CA-C-N | 9.26  | 139.22      | 121.54   |
| 10  | C24   | 1057 | THR  | C-N-CA | 9.26  | 139.22      | 121.54   |
| 18  | B     | 1962 | PRO  | O-C-N  | -9.26 | 112.36      | 123.01   |
| 11  | A32   | 555  | HIS  | O-C-N  | -9.25 | 108.66      | 122.81   |
| 7   | Q     | 89   | GLY  | CA-C-N | 9.25  | 139.53      | 121.41   |
| 7   | Q     | 89   | GLY  | C-N-CA | 9.25  | 139.53      | 121.41   |
| 10  | C     | 1057 | THR  | CA-C-N | 9.25  | 139.20      | 121.54   |
| 10  | C     | 1057 | THR  | C-N-CA | 9.25  | 139.20      | 121.54   |
| 10  | C     | 1223 | ASP  | O-C-N  | -9.25 | 112.51      | 122.96   |
| 7   | Q8    | 89   | GLY  | CA-C-N | 9.24  | 139.52      | 121.41   |
| 7   | Q8    | 89   | GLY  | C-N-CA | 9.24  | 139.52      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 1223 | ASP  | O-C-N  | -9.24 | 112.52      | 122.96   |
| 20  | E8    | 443  | ASP  | O-C-N  | -9.24 | 110.31      | 122.59   |
| 10  | C24   | 1223 | ASP  | O-C-N  | -9.23 | 112.53      | 122.96   |
| 10  | C8    | 1223 | ASP  | O-C-N  | -9.23 | 112.53      | 122.96   |
| 20  | E8    | 439  | MET  | O-C-N  | -9.23 | 110.31      | 122.59   |
| 20  | E     | 439  | MET  | O-C-N  | -9.23 | 110.32      | 122.59   |
| 11  | A16   | 555  | HIS  | O-C-N  | -9.23 | 108.69      | 122.81   |
| 23  | J16   | 678  | GLY  | CA-C-N | -9.22 | 107.29      | 122.32   |
| 23  | J16   | 678  | GLY  | C-N-CA | -9.22 | 107.29      | 122.32   |
| 11  | A40   | 555  | HIS  | O-C-N  | -9.22 | 108.70      | 122.81   |
| 11  | A24   | 555  | HIS  | O-C-N  | -9.22 | 108.71      | 122.81   |
| 1   | R8    | 1209 | GLY  | O-C-N  | -9.21 | 110.72      | 122.70   |
| 20  | E     | 443  | ASP  | O-C-N  | -9.21 | 110.34      | 122.59   |
| 23  | J24   | 678  | GLY  | CA-C-N | -9.21 | 107.30      | 122.32   |
| 23  | J24   | 678  | GLY  | C-N-CA | -9.21 | 107.30      | 122.32   |
| 1   | R16   | 1142 | GLY  | O-C-N  | -9.21 | 108.54      | 122.26   |
| 23  | J32   | 678  | GLY  | CA-C-N | -9.21 | 107.31      | 122.32   |
| 23  | J32   | 678  | GLY  | C-N-CA | -9.21 | 107.31      | 122.32   |
| 10  | C8    | 508  | ILE  | O-C-N  | -9.21 | 113.44      | 123.20   |
| 18  | B8    | 685  | SER  | O-C-N  | -9.21 | 110.34      | 122.59   |
| 1   | R     | 1142 | GLY  | O-C-N  | -9.20 | 108.55      | 122.26   |
| 9   | K8    | 893  | ASN  | O-C-N  | -9.20 | 110.50      | 122.56   |
| 20  | E     | 423  | PRO  | O-C-N  | -9.20 | 110.22      | 122.64   |
| 12  | A     | 555  | HIS  | O-C-N  | -9.20 | 108.74      | 122.81   |
| 23  | J8    | 678  | GLY  | CA-C-N | -9.20 | 107.33      | 122.32   |
| 23  | J8    | 678  | GLY  | C-N-CA | -9.20 | 107.33      | 122.32   |
| 9   | K8    | 1088 | ASP  | CA-C-N | 9.19  | 139.10      | 121.54   |
| 9   | K8    | 1088 | ASP  | C-N-CA | 9.19  | 139.10      | 121.54   |
| 18  | B     | 685  | SER  | O-C-N  | -9.19 | 110.36      | 122.59   |
| 1   | R16   | 1209 | GLY  | O-C-N  | -9.19 | 110.75      | 122.70   |
| 12  | A48   | 555  | HIS  | O-C-N  | -9.19 | 108.75      | 122.81   |
| 7   | Q16   | 89   | GLY  | CA-C-N | 9.19  | 139.42      | 121.41   |
| 7   | Q16   | 89   | GLY  | C-N-CA | 9.19  | 139.42      | 121.41   |
| 9   | K     | 1088 | ASP  | CA-C-N | 9.18  | 139.08      | 121.54   |
| 9   | K     | 1088 | ASP  | C-N-CA | 9.18  | 139.08      | 121.54   |
| 1   | R     | 1209 | GLY  | O-C-N  | -9.18 | 110.76      | 122.70   |
| 9   | K     | 893  | ASN  | O-C-N  | -9.18 | 110.53      | 122.56   |
| 20  | E8    | 423  | PRO  | O-C-N  | -9.18 | 110.24      | 122.64   |
| 10  | C32   | 676  | ARG  | O-C-N  | -9.18 | 108.80      | 122.39   |
| 10  | C16   | 679  | ARG  | O-C-N  | -9.18 | 112.90      | 123.27   |
| 13  | V     | 873  | GLY  | CA-C-N | 9.18  | 130.90      | 120.53   |
| 13  | V     | 873  | GLY  | C-N-CA | 9.18  | 130.90      | 120.53   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 676  | ARG  | O-C-N  | -9.17 | 108.82      | 122.39   |
| 1   | R8    | 1142 | GLY  | O-C-N  | -9.17 | 108.60      | 122.26   |
| 18  | B8    | 675  | SER  | O-C-N  | -9.17 | 112.40      | 122.12   |
| 10  | C24   | 676  | ARG  | O-C-N  | -9.16 | 108.83      | 122.39   |
| 10  | C     | 679  | ARG  | O-C-N  | -9.15 | 112.93      | 123.27   |
| 10  | C8    | 679  | ARG  | O-C-N  | -9.14 | 112.94      | 123.27   |
| 18  | B     | 675  | SER  | O-C-N  | -9.14 | 112.43      | 122.12   |
| 10  | C24   | 679  | ARG  | O-C-N  | -9.12 | 112.96      | 123.27   |
| 18  | B8    | 1669 | PRO  | O-C-N  | -9.13 | 110.32      | 122.64   |
| 10  | C8    | 676  | ARG  | O-C-N  | -9.12 | 108.89      | 122.39   |
| 10  | C32   | 679  | ARG  | O-C-N  | -9.12 | 112.97      | 123.27   |
| 18  | B     | 1669 | PRO  | O-C-N  | -9.11 | 110.35      | 122.64   |
| 20  | E8    | 347  | PRO  | CA-C-N | 9.09  | 131.20      | 119.84   |
| 20  | E8    | 347  | PRO  | C-N-CA | 9.09  | 131.20      | 119.84   |
| 10  | C     | 676  | ARG  | O-C-N  | -9.09 | 108.94      | 122.39   |
| 20  | E8    | 347  | PRO  | O-C-N  | -9.08 | 110.75      | 121.46   |
| 12  | A48   | 461  | VAL  | O-C-N  | -9.07 | 110.89      | 122.32   |
| 10  | C16   | 1782 | SER  | CA-C-N | 9.07  | 135.60      | 121.19   |
| 10  | C16   | 1782 | SER  | C-N-CA | 9.07  | 135.60      | 121.19   |
| 20  | E     | 347  | PRO  | CA-C-N | 9.06  | 131.17      | 119.84   |
| 20  | E     | 347  | PRO  | C-N-CA | 9.06  | 131.17      | 119.84   |
| 10  | C32   | 635  | GLN  | O-C-N  | -9.06 | 110.53      | 122.59   |
| 11  | A24   | 461  | VAL  | O-C-N  | -9.06 | 110.90      | 122.32   |
| 10  | C32   | 1782 | SER  | CA-C-N | 9.06  | 135.59      | 121.19   |
| 10  | C32   | 1782 | SER  | C-N-CA | 9.06  | 135.59      | 121.19   |
| 9   | K     | 1066 | ASP  | O-C-N  | -9.04 | 110.56      | 122.59   |
| 9   | K8    | 717  | ARG  | O-C-N  | -9.04 | 111.84      | 122.15   |
| 12  | A     | 461  | VAL  | O-C-N  | -9.04 | 110.93      | 122.32   |
| 20  | E     | 347  | PRO  | O-C-N  | -9.04 | 110.79      | 121.46   |
| 10  | C16   | 635  | GLN  | O-C-N  | -9.04 | 110.57      | 122.59   |
| 10  | C24   | 1782 | SER  | CA-C-N | 9.04  | 135.56      | 121.19   |
| 10  | C24   | 1782 | SER  | C-N-CA | 9.04  | 135.56      | 121.19   |
| 11  | A32   | 461  | VAL  | O-C-N  | -9.03 | 110.94      | 122.32   |
| 2   | M16   | 336  | SER  | O-C-N  | -9.03 | 111.66      | 122.22   |
| 11  | A16   | 464  | GLY  | O-C-N  | -9.02 | 113.44      | 122.19   |
| 18  | B8    | 979  | VAL  | O-C-N  | -9.02 | 111.29      | 122.57   |
| 9   | K     | 717  | ARG  | O-C-N  | -9.02 | 111.87      | 122.15   |
| 12  | A     | 309  | VAL  | O-C-N  | -9.02 | 110.42      | 122.14   |
| 10  | C     | 635  | GLN  | O-C-N  | -9.02 | 110.60      | 122.59   |
| 9   | K8    | 1066 | ASP  | O-C-N  | -9.01 | 110.60      | 122.59   |
| 1   | R     | 1382 | LYS  | CA-C-N | -9.01 | 110.30      | 123.00   |
| 1   | R     | 1382 | LYS  | C-N-CA | -9.01 | 110.30      | 123.00   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 979  | VAL  | O-C-N  | -9.01 | 111.31      | 122.57   |
| 18  | B8    | 1797 | LEU  | CA-C-N | -9.01 | 109.73      | 120.72   |
| 18  | B8    | 1797 | LEU  | C-N-CA | -9.01 | 109.73      | 120.72   |
| 2   | M16   | 352  | LYS  | O-C-N  | -9.01 | 110.61      | 122.59   |
| 18  | B     | 1797 | LEU  | CA-C-N | -9.01 | 109.73      | 120.72   |
| 18  | B     | 1797 | LEU  | C-N-CA | -9.01 | 109.73      | 120.72   |
| 2   | M8    | 814  | PRO  | CA-C-N | -9.00 | 110.15      | 122.30   |
| 2   | M8    | 814  | PRO  | C-N-CA | -9.00 | 110.15      | 122.30   |
| 10  | C24   | 635  | GLN  | O-C-N  | -9.00 | 110.61      | 122.59   |
| 5   | P16   | 144  | THR  | CA-C-N | -8.99 | 105.79      | 121.97   |
| 5   | P16   | 144  | THR  | C-N-CA | -8.99 | 105.79      | 121.97   |
| 12  | A48   | 309  | VAL  | O-C-N  | -8.99 | 110.46      | 122.14   |
| 10  | C     | 1782 | SER  | CA-C-N | 8.98  | 135.47      | 121.19   |
| 10  | C     | 1782 | SER  | C-N-CA | 8.98  | 135.47      | 121.19   |
| 2   | M16   | 814  | PRO  | CA-C-N | -8.98 | 110.17      | 122.30   |
| 2   | M16   | 814  | PRO  | C-N-CA | -8.98 | 110.17      | 122.30   |
| 2   | M     | 814  | PRO  | CA-C-N | -8.98 | 110.18      | 122.30   |
| 2   | M     | 814  | PRO  | C-N-CA | -8.98 | 110.18      | 122.30   |
| 10  | C8    | 1782 | SER  | CA-C-N | 8.98  | 135.47      | 121.19   |
| 10  | C8    | 1782 | SER  | C-N-CA | 8.98  | 135.47      | 121.19   |
| 11  | A40   | 464  | GLY  | O-C-N  | -8.97 | 113.49      | 122.19   |
| 18  | B8    | 116  | THR  | O-C-N  | -8.97 | 111.28      | 122.68   |
| 2   | M     | 352  | LYS  | O-C-N  | -8.97 | 110.66      | 122.59   |
| 11  | A32   | 464  | GLY  | O-C-N  | -8.97 | 113.49      | 122.19   |
| 18  | B     | 116  | THR  | O-C-N  | -8.97 | 111.29      | 122.68   |
| 2   | M8    | 336  | SER  | O-C-N  | -8.96 | 111.73      | 122.22   |
| 11  | A40   | 461  | VAL  | O-C-N  | -8.96 | 111.02      | 122.32   |
| 2   | M8    | 352  | LYS  | O-C-N  | -8.96 | 110.67      | 122.59   |
| 10  | C24   | 1661 | LEU  | O-C-N  | -8.96 | 110.67      | 122.59   |
| 11  | A16   | 461  | VAL  | O-C-N  | -8.96 | 111.03      | 122.32   |
| 5   | P8    | 144  | THR  | CA-C-N | -8.96 | 105.85      | 121.97   |
| 5   | P8    | 144  | THR  | C-N-CA | -8.96 | 105.85      | 121.97   |
| 1   | R16   | 1382 | LYS  | CA-C-N | -8.95 | 110.39      | 123.00   |
| 1   | R16   | 1382 | LYS  | C-N-CA | -8.95 | 110.39      | 123.00   |
| 5   | P     | 144  | THR  | CA-C-N | -8.95 | 105.86      | 121.97   |
| 5   | P     | 144  | THR  | C-N-CA | -8.95 | 105.86      | 121.97   |
| 10  | C8    | 1163 | LEU  | O-C-N  | -8.94 | 93.08       | 122.06   |
| 1   | R8    | 1382 | LYS  | CA-C-N | -8.94 | 110.39      | 123.00   |
| 1   | R8    | 1382 | LYS  | C-N-CA | -8.94 | 110.39      | 123.00   |
| 10  | C     | 1163 | LEU  | O-C-N  | -8.94 | 93.09       | 122.06   |
| 18  | B8    | 1478 | MET  | O-C-N  | -8.93 | 110.08      | 122.41   |
| 11  | A40   | 309  | VAL  | O-C-N  | -8.93 | 110.53      | 122.14   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 1163 | LEU  | O-C-N  | -8.93 | 93.13       | 122.06   |
| 10  | C24   | 1163 | LEU  | O-C-N  | -8.93 | 93.12       | 122.06   |
| 10  | C32   | 1163 | LEU  | O-C-N  | -8.93 | 93.12       | 122.06   |
| 10  | C     | 1661 | LEU  | O-C-N  | -8.92 | 110.73      | 122.59   |
| 5   | P16   | 595  | SER  | O-C-N  | -8.91 | 110.74      | 122.59   |
| 10  | C32   | 1661 | LEU  | O-C-N  | -8.91 | 110.74      | 122.59   |
| 2   | M     | 336  | SER  | O-C-N  | -8.91 | 111.80      | 122.22   |
| 18  | B     | 1478 | MET  | O-C-N  | -8.90 | 110.12      | 122.41   |
| 9   | K8    | 1214 | TYR  | O-C-N  | -8.90 | 111.41      | 122.35   |
| 11  | A16   | 309  | VAL  | O-C-N  | -8.90 | 110.58      | 122.14   |
| 9   | K8    | 1059 | ARG  | CA-C-N | 8.89  | 134.16      | 120.82   |
| 9   | K8    | 1059 | ARG  | C-N-CA | 8.89  | 134.16      | 120.82   |
| 11  | A24   | 309  | VAL  | O-C-N  | -8.89 | 110.58      | 122.14   |
| 9   | K     | 1059 | ARG  | CA-C-N | 8.88  | 134.15      | 120.82   |
| 9   | K     | 1059 | ARG  | C-N-CA | 8.88  | 134.15      | 120.82   |
| 5   | P8    | 595  | SER  | O-C-N  | -8.88 | 110.78      | 122.59   |
| 18  | B     | 617  | ASP  | O-C-N  | -8.88 | 110.41      | 122.48   |
| 18  | B8    | 617  | ASP  | O-C-N  | -8.87 | 110.41      | 122.48   |
| 1   | R8    | 1191 | LYS  | O-C-N  | -8.87 | 111.91      | 122.11   |
| 5   | P     | 595  | SER  | O-C-N  | -8.87 | 110.79      | 122.59   |
| 1   | R     | 1191 | LYS  | O-C-N  | -8.87 | 111.91      | 122.11   |
| 18  | B8    | 679  | ASP  | CA-C-N | -8.87 | 107.79      | 120.82   |
| 18  | B8    | 679  | ASP  | C-N-CA | -8.87 | 107.79      | 120.82   |
| 1   | R16   | 1191 | LYS  | O-C-N  | -8.86 | 111.92      | 122.11   |
| 9   | K     | 1214 | TYR  | O-C-N  | -8.86 | 111.45      | 122.35   |
| 10  | C16   | 1661 | LEU  | O-C-N  | -8.85 | 110.81      | 122.59   |
| 10  | C8    | 280  | SER  | CA-C-N | 8.85  | 138.44      | 121.54   |
| 10  | C8    | 280  | SER  | C-N-CA | 8.85  | 138.44      | 121.54   |
| 12  | A48   | 464  | GLY  | O-C-N  | -8.85 | 113.61      | 122.19   |
| 11  | A32   | 309  | VAL  | O-C-N  | -8.85 | 110.64      | 122.14   |
| 18  | B     | 679  | ASP  | CA-C-N | -8.85 | 107.81      | 120.82   |
| 18  | B     | 679  | ASP  | C-N-CA | -8.85 | 107.81      | 120.82   |
| 9   | K     | 1119 | ASN  | O-C-N  | -8.84 | 110.73      | 122.57   |
| 10  | C32   | 280  | SER  | CA-C-N | 8.84  | 138.42      | 121.54   |
| 10  | C32   | 280  | SER  | C-N-CA | 8.84  | 138.42      | 121.54   |
| 11  | A24   | 464  | GLY  | O-C-N  | -8.83 | 113.62      | 122.19   |
| 5   | P16   | 9    | GLY  | CA-C-N | 8.83  | 138.72      | 121.41   |
| 5   | P16   | 9    | GLY  | C-N-CA | 8.83  | 138.72      | 121.41   |
| 9   | K8    | 716  | ALA  | O-C-N  | -8.82 | 112.10      | 122.15   |
| 10  | C16   | 1788 | HIS  | CA-C-N | 8.82  | 132.94      | 120.42   |
| 10  | C16   | 1788 | HIS  | C-N-CA | 8.82  | 132.94      | 120.42   |
| 10  | C24   | 280  | SER  | CA-C-N | 8.82  | 138.38      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 280  | SER  | C-N-CA | 8.82  | 138.38      | 121.54   |
| 10  | C24   | 1052 | PHE  | O-C-N  | -8.82 | 110.76      | 122.22   |
| 1   | R     | 1121 | ARG  | CA-C-N | 8.81  | 136.88      | 123.05   |
| 1   | R     | 1121 | ARG  | C-N-CA | 8.81  | 136.88      | 123.05   |
| 9   | K8    | 1119 | ASN  | O-C-N  | -8.81 | 110.76      | 122.57   |
| 1   | R16   | 1121 | ARG  | CA-C-N | 8.80  | 136.87      | 123.05   |
| 1   | R16   | 1121 | ARG  | C-N-CA | 8.80  | 136.87      | 123.05   |
| 10  | C32   | 1054 | ARG  | O-C-N  | -8.81 | 111.86      | 122.96   |
| 5   | P     | 9    | GLY  | CA-C-N | 8.80  | 138.66      | 121.41   |
| 5   | P     | 9    | GLY  | C-N-CA | 8.80  | 138.66      | 121.41   |
| 1   | R8    | 1121 | ARG  | CA-C-N | 8.79  | 136.86      | 123.05   |
| 1   | R8    | 1121 | ARG  | C-N-CA | 8.79  | 136.86      | 123.05   |
| 10  | C32   | 1788 | HIS  | CA-C-N | 8.79  | 132.91      | 120.42   |
| 10  | C32   | 1788 | HIS  | C-N-CA | 8.79  | 132.91      | 120.42   |
| 12  | A     | 464  | GLY  | O-C-N  | -8.79 | 113.66      | 122.19   |
| 10  | C     | 1130 | SER  | O-C-N  | -8.79 | 110.89      | 122.59   |
| 10  | C16   | 280  | SER  | CA-C-N | 8.79  | 138.33      | 121.54   |
| 10  | C16   | 280  | SER  | C-N-CA | 8.79  | 138.33      | 121.54   |
| 10  | C16   | 1054 | ARG  | O-C-N  | -8.79 | 111.88      | 122.96   |
| 10  | C     | 280  | SER  | CA-C-N | 8.79  | 138.33      | 121.54   |
| 10  | C     | 280  | SER  | C-N-CA | 8.79  | 138.33      | 121.54   |
| 10  | C16   | 1130 | SER  | O-C-N  | -8.79 | 110.90      | 122.59   |
| 10  | C8    | 1130 | SER  | O-C-N  | -8.78 | 110.91      | 122.59   |
| 10  | C8    | 1054 | ARG  | O-C-N  | -8.78 | 111.90      | 122.96   |
| 10  | C32   | 1052 | PHE  | O-C-N  | -8.78 | 110.81      | 122.22   |
| 5   | P8    | 9    | GLY  | CA-C-N | 8.78  | 138.61      | 121.41   |
| 5   | P8    | 9    | GLY  | C-N-CA | 8.78  | 138.61      | 121.41   |
| 10  | C24   | 1788 | HIS  | CA-C-N | 8.78  | 132.88      | 120.42   |
| 10  | C24   | 1788 | HIS  | C-N-CA | 8.78  | 132.88      | 120.42   |
| 10  | C8    | 1052 | PHE  | O-C-N  | -8.77 | 110.82      | 122.22   |
| 10  | C8    | 1788 | HIS  | CA-C-N | 8.77  | 132.88      | 120.42   |
| 10  | C8    | 1788 | HIS  | C-N-CA | 8.77  | 132.88      | 120.42   |
| 18  | B     | 1679 | ARG  | O-C-N  | -8.77 | 110.93      | 122.59   |
| 5   | P16   | 1    | MET  | CA-C-N | 8.77  | 130.80      | 119.84   |
| 5   | P16   | 1    | MET  | C-N-CA | 8.77  | 130.80      | 119.84   |
| 10  | C     | 1054 | ARG  | O-C-N  | -8.76 | 111.92      | 122.96   |
| 10  | C8    | 1502 | ARG  | CA-C-N | -8.76 | 106.19      | 121.97   |
| 10  | C8    | 1502 | ARG  | C-N-CA | -8.76 | 106.19      | 121.97   |
| 9   | K     | 716  | ALA  | O-C-N  | -8.76 | 112.17      | 122.15   |
| 10  | C     | 1502 | ARG  | CA-C-N | -8.75 | 106.21      | 121.97   |
| 10  | C     | 1502 | ARG  | C-N-CA | -8.75 | 106.21      | 121.97   |
| 10  | C     | 1788 | HIS  | CA-C-N | 8.75  | 132.85      | 120.42   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C     | 1788 | HIS  | C-N-CA | 8.75  | 132.85      | 120.42   |
| 10  | C8    | 1079 | THR  | O-C-N  | -8.75 | 110.95      | 122.59   |
| 10  | C24   | 1054 | ARG  | O-C-N  | -8.75 | 111.94      | 122.96   |
| 14  | W     | 597  | ARG  | O-C-N  | -8.74 | 110.85      | 122.57   |
| 10  | C32   | 1130 | SER  | O-C-N  | -8.74 | 110.96      | 122.59   |
| 10  | C24   | 1130 | SER  | O-C-N  | -8.74 | 110.97      | 122.59   |
| 18  | B8    | 1679 | ARG  | O-C-N  | -8.74 | 110.97      | 122.59   |
| 10  | C8    | 1064 | PHE  | O-C-N  | -8.73 | 110.97      | 122.59   |
| 19  | 4     | 60   | GLN  | CA-C-N | -8.73 | 104.87      | 121.54   |
| 19  | 4     | 60   | GLN  | C-N-CA | -8.73 | 104.87      | 121.54   |
| 5   | P8    | 8    | SER  | O-C-N  | -8.72 | 110.99      | 122.59   |
| 10  | C24   | 1502 | ARG  | CA-C-N | -8.72 | 106.27      | 121.97   |
| 10  | C24   | 1502 | ARG  | C-N-CA | -8.72 | 106.27      | 121.97   |
| 19  | 48    | 60   | GLN  | CA-C-N | -8.72 | 104.88      | 121.54   |
| 19  | 48    | 60   | GLN  | C-N-CA | -8.72 | 104.88      | 121.54   |
| 5   | P     | 8    | SER  | O-C-N  | -8.72 | 110.99      | 122.59   |
| 10  | C32   | 1064 | PHE  | O-C-N  | -8.72 | 111.00      | 122.59   |
| 10  | C32   | 1502 | ARG  | CA-C-N | -8.72 | 106.28      | 121.97   |
| 10  | C32   | 1502 | ARG  | C-N-CA | -8.72 | 106.28      | 121.97   |
| 10  | C24   | 1079 | THR  | O-C-N  | -8.71 | 111.00      | 122.59   |
| 10  | C16   | 1052 | PHE  | O-C-N  | -8.71 | 110.90      | 122.22   |
| 10  | C24   | 1064 | PHE  | O-C-N  | -8.71 | 111.01      | 122.59   |
| 14  | W     | 592  | ALA  | O-C-N  | -8.71 | 109.72      | 122.43   |
| 10  | C     | 1052 | PHE  | O-C-N  | -8.70 | 110.91      | 122.22   |
| 10  | C     | 1079 | THR  | O-C-N  | -8.69 | 111.03      | 122.59   |
| 5   | P     | 1    | MET  | CA-C-N | 8.69  | 130.71      | 119.84   |
| 5   | P     | 1    | MET  | C-N-CA | 8.69  | 130.71      | 119.84   |
| 10  | C16   | 1064 | PHE  | O-C-N  | -8.69 | 111.03      | 122.59   |
| 11  | A32   | 159  | LYS  | O-C-N  | -8.69 | 112.18      | 122.87   |
| 5   | P8    | 1    | MET  | CA-C-N | 8.69  | 130.70      | 119.84   |
| 5   | P8    | 1    | MET  | C-N-CA | 8.69  | 130.70      | 119.84   |
| 10  | C16   | 1502 | ARG  | CA-C-N | -8.69 | 106.34      | 121.97   |
| 10  | C16   | 1502 | ARG  | C-N-CA | -8.69 | 106.34      | 121.97   |
| 5   | P16   | 8    | SER  | O-C-N  | -8.68 | 111.04      | 122.59   |
| 10  | C24   | 1444 | GLY  | O-C-N  | -8.68 | 111.41      | 122.70   |
| 10  | C     | 1064 | PHE  | O-C-N  | -8.68 | 111.04      | 122.59   |
| 7   | Q16   | 94   | SER  | O-C-N  | -8.68 | 111.66      | 122.68   |
| 10  | C     | 1444 | GLY  | O-C-N  | -8.68 | 111.42      | 122.70   |
| 18  | B8    | 977  | SER  | O-C-N  | -8.67 | 112.80      | 122.08   |
| 10  | C8    | 712  | LEU  | CA-C-N | 8.66  | 132.76      | 120.28   |
| 10  | C8    | 712  | LEU  | C-N-CA | 8.66  | 132.76      | 120.28   |
| 11  | A16   | 159  | LYS  | O-C-N  | -8.66 | 112.22      | 122.87   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13  | V     | 809  | THR  | O-C-N  | 8.65  | 131.29      | 122.12   |
| 10  | C8    | 1444 | GLY  | O-C-N  | -8.65 | 111.45      | 122.70   |
| 7   | Q     | 94   | SER  | O-C-N  | -8.65 | 111.70      | 122.68   |
| 7   | Q8    | 94   | SER  | O-C-N  | -8.64 | 111.70      | 122.68   |
| 10  | C16   | 1079 | THR  | O-C-N  | -8.64 | 111.10      | 122.59   |
| 18  | B     | 977  | SER  | O-C-N  | -8.64 | 112.84      | 122.08   |
| 10  | C32   | 1444 | GLY  | O-C-N  | -8.64 | 111.47      | 122.70   |
| 9   | K     | 719  | GLY  | O-C-N  | -8.63 | 111.48      | 122.70   |
| 10  | C32   | 1079 | THR  | O-C-N  | -8.63 | 111.12      | 122.59   |
| 19  | 48    | 191  | GLY  | CA-C-N | -8.61 | 107.42      | 122.07   |
| 19  | 48    | 191  | GLY  | C-N-CA | -8.61 | 107.42      | 122.07   |
| 10  | C16   | 1444 | GLY  | O-C-N  | -8.61 | 111.51      | 122.70   |
| 10  | C16   | 712  | LEU  | CA-C-N | 8.60  | 132.66      | 120.28   |
| 10  | C16   | 712  | LEU  | C-N-CA | 8.60  | 132.66      | 120.28   |
| 18  | B     | 1123 | ASN  | CA-C-N | -8.60 | 104.56      | 121.41   |
| 18  | B     | 1123 | ASN  | C-N-CA | -8.60 | 104.56      | 121.41   |
| 5   | P     | 6    | SER  | O-C-N  | -8.59 | 111.16      | 122.59   |
| 19  | 4     | 191  | GLY  | CA-C-N | -8.59 | 107.46      | 122.07   |
| 19  | 4     | 191  | GLY  | C-N-CA | -8.59 | 107.46      | 122.07   |
| 21  | H16   | 326  | GLY  | O-C-N  | -8.59 | 111.53      | 122.70   |
| 10  | C32   | 712  | LEU  | CA-C-N | 8.59  | 132.65      | 120.28   |
| 10  | C32   | 712  | LEU  | C-N-CA | 8.59  | 132.65      | 120.28   |
| 5   | P8    | 6    | SER  | O-C-N  | -8.59 | 111.17      | 122.59   |
| 10  | C     | 1779 | GLU  | O-C-N  | -8.59 | 111.05      | 122.38   |
| 10  | C24   | 712  | LEU  | CA-C-N | 8.58  | 132.64      | 120.28   |
| 10  | C24   | 712  | LEU  | C-N-CA | 8.58  | 132.64      | 120.28   |
| 10  | C     | 712  | LEU  | CA-C-N | 8.58  | 132.64      | 120.28   |
| 10  | C     | 712  | LEU  | C-N-CA | 8.58  | 132.64      | 120.28   |
| 5   | P16   | 6    | SER  | O-C-N  | -8.58 | 111.18      | 122.59   |
| 9   | K8    | 719  | GLY  | O-C-N  | -8.58 | 111.55      | 122.70   |
| 18  | B8    | 1123 | ASN  | CA-C-N | -8.58 | 104.60      | 121.41   |
| 18  | B8    | 1123 | ASN  | C-N-CA | -8.58 | 104.60      | 121.41   |
| 10  | C32   | 1779 | GLU  | O-C-N  | -8.58 | 111.06      | 122.38   |
| 21  | H24   | 326  | GLY  | O-C-N  | -8.56 | 111.57      | 122.70   |
| 1   | R8    | 1207 | PRO  | O-C-N  | -8.55 | 111.09      | 122.64   |
| 1   | R16   | 1121 | ARG  | O-C-N  | -8.55 | 110.27      | 122.41   |
| 10  | C8    | 1779 | GLU  | O-C-N  | -8.55 | 111.10      | 122.38   |
| 18  | B     | 1784 | GLY  | O-C-N  | -8.55 | 111.59      | 122.70   |
| 1   | R     | 1207 | PRO  | O-C-N  | -8.53 | 111.12      | 122.64   |
| 1   | R8    | 1121 | ARG  | O-C-N  | -8.54 | 110.29      | 122.41   |
| 2   | M16   | 342  | VAL  | O-C-N  | -8.54 | 111.90      | 122.57   |
| 2   | M8    | 342  | VAL  | O-C-N  | -8.53 | 111.91      | 122.57   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | R16   | 1146 | ASP  | O-C-N      | -8.53 | 112.82      | 123.06   |
| 2   | M     | 342  | VAL  | O-C-N      | -8.53 | 111.91      | 122.57   |
| 10  | C16   | 1779 | GLU  | O-C-N      | -8.53 | 111.12      | 122.38   |
| 1   | R     | 1121 | ARG  | O-C-N      | -8.52 | 110.31      | 122.41   |
| 18  | B     | 1066 | ASP  | CA-C-N     | -8.52 | 108.41      | 121.02   |
| 18  | B     | 1066 | ASP  | C-N-CA     | -8.52 | 108.41      | 121.02   |
| 5   | P     | 2    | PRO  | O-C-N      | -8.52 | 111.14      | 122.64   |
| 1   | R     | 1187 | ARG  | O-C-N      | -8.52 | 111.27      | 122.59   |
| 5   | P8    | 2    | PRO  | O-C-N      | -8.52 | 111.14      | 122.64   |
| 20  | E8    | 206  | GLY  | CA-C-N     | 8.51  | 137.80      | 121.54   |
| 20  | E8    | 206  | GLY  | C-N-CA     | 8.51  | 137.80      | 121.54   |
| 1   | R     | 1146 | ASP  | O-C-N      | -8.51 | 112.85      | 123.06   |
| 10  | C24   | 1779 | GLU  | O-C-N      | -8.51 | 111.15      | 122.38   |
| 1   | R16   | 1207 | PRO  | O-C-N      | -8.51 | 111.15      | 122.64   |
| 20  | E     | 206  | GLY  | CA-C-N     | 8.51  | 137.79      | 121.54   |
| 20  | E     | 206  | GLY  | C-N-CA     | 8.51  | 137.79      | 121.54   |
| 18  | B     | 1228 | SER  | O-C-N      | -8.50 | 111.28      | 122.59   |
| 21  | H8    | 326  | GLY  | O-C-N      | -8.50 | 111.64      | 122.70   |
| 1   | R8    | 1146 | ASP  | O-C-N      | -8.50 | 112.86      | 123.06   |
| 18  | B8    | 1784 | GLY  | O-C-N      | -8.49 | 111.66      | 122.70   |
| 2   | M8    | 389  | SER  | O-C-N      | -8.48 | 111.73      | 123.01   |
| 9   | K     | 1140 | GLN  | CA-C-N     | 8.47  | 138.02      | 121.41   |
| 9   | K     | 1140 | GLN  | C-N-CA     | 8.47  | 138.02      | 121.41   |
| 21  | H     | 326  | GLY  | O-C-N      | -8.47 | 111.68      | 122.70   |
| 18  | B     | 676  | ASP  | CA-C-N     | -8.47 | 106.46      | 122.13   |
| 18  | B     | 676  | ASP  | C-N-CA     | -8.47 | 106.46      | 122.13   |
| 2   | M     | 389  | SER  | O-C-N      | -8.47 | 111.75      | 123.01   |
| 18  | B8    | 676  | ASP  | CA-C-N     | -8.47 | 106.46      | 122.13   |
| 18  | B8    | 676  | ASP  | C-N-CA     | -8.47 | 106.46      | 122.13   |
| 1   | R8    | 1187 | ARG  | O-C-N      | -8.47 | 111.33      | 122.59   |
| 4   | T16   | 160  | HIS  | CG-ND1-CE1 | 8.47  | 123.69      | 109.30   |
| 10  | C8    | 1032 | THR  | O-C-N      | -8.47 | 110.69      | 122.37   |
| 1   | R16   | 1187 | ARG  | O-C-N      | -8.46 | 111.33      | 122.59   |
| 18  | B8    | 1228 | SER  | O-C-N      | -8.47 | 111.33      | 122.59   |
| 10  | C16   | 1541 | PHE  | CA-C-N     | -8.46 | 105.37      | 121.54   |
| 10  | C16   | 1541 | PHE  | C-N-CA     | -8.46 | 105.37      | 121.54   |
| 9   | K8    | 1140 | GLN  | CA-C-N     | 8.46  | 138.00      | 121.41   |
| 9   | K8    | 1140 | GLN  | C-N-CA     | 8.46  | 138.00      | 121.41   |
| 10  | C8    | 734  | LEU  | CA-C-N     | 8.46  | 128.96      | 119.32   |
| 10  | C8    | 734  | LEU  | C-N-CA     | 8.46  | 128.96      | 119.32   |
| 4   | T8    | 160  | HIS  | CG-ND1-CE1 | 8.46  | 123.67      | 109.30   |
| 1   | R16   | 1246 | LYS  | O-C-N      | 8.45  | 129.60      | 121.66   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14  | W     | 701  | LEU  | CA-C-N     | 8.45  | 130.40      | 119.84   |
| 14  | W     | 701  | LEU  | C-N-CA     | 8.45  | 130.40      | 119.84   |
| 10  | C16   | 734  | LEU  | CA-C-N     | 8.45  | 128.95      | 119.32   |
| 10  | C16   | 734  | LEU  | C-N-CA     | 8.45  | 128.95      | 119.32   |
| 10  | C16   | 1032 | THR  | O-C-N      | -8.45 | 110.71      | 122.37   |
| 10  | C24   | 1541 | PHE  | CA-C-N     | -8.45 | 105.41      | 121.54   |
| 10  | C24   | 1541 | PHE  | C-N-CA     | -8.45 | 105.41      | 121.54   |
| 2   | M16   | 389  | SER  | O-C-N      | -8.44 | 111.79      | 123.01   |
| 5   | P16   | 2    | PRO  | O-C-N      | -8.44 | 111.25      | 122.64   |
| 10  | C32   | 1541 | PHE  | CA-C-N     | -8.44 | 105.42      | 121.54   |
| 10  | C32   | 1541 | PHE  | C-N-CA     | -8.44 | 105.42      | 121.54   |
| 10  | C     | 1032 | THR  | O-C-N      | -8.44 | 110.73      | 122.37   |
| 10  | C24   | 1032 | THR  | O-C-N      | -8.43 | 110.73      | 122.37   |
| 10  | C8    | 1541 | PHE  | CA-C-N     | -8.43 | 105.43      | 121.54   |
| 10  | C8    | 1541 | PHE  | C-N-CA     | -8.43 | 105.43      | 121.54   |
| 1   | R8    | 1246 | LYS  | O-C-N      | 8.43  | 129.58      | 121.66   |
| 18  | B8    | 298  | THR  | O-C-N      | -8.43 | 111.38      | 122.59   |
| 18  | B8    | 676  | ASP  | O-C-N      | -8.43 | 112.36      | 122.22   |
| 14  | W     | 610  | PRO  | CA-C-N     | 8.42  | 132.41      | 120.28   |
| 14  | W     | 610  | PRO  | C-N-CA     | 8.42  | 132.41      | 120.28   |
| 10  | C     | 734  | LEU  | CA-C-N     | 8.42  | 128.91      | 119.32   |
| 10  | C     | 734  | LEU  | C-N-CA     | 8.42  | 128.91      | 119.32   |
| 9   | K8    | 891  | GLU  | CA-C-N     | 8.41  | 137.61      | 121.54   |
| 9   | K8    | 891  | GLU  | C-N-CA     | 8.41  | 137.61      | 121.54   |
| 1   | R     | 1246 | LYS  | O-C-N      | 8.41  | 129.57      | 121.66   |
| 18  | B8    | 1811 | PRO  | O-C-N      | -8.41 | 113.01      | 123.10   |
| 2   | M16   | 551  | GLU  | CA-C-N     | 8.40  | 137.82      | 121.18   |
| 2   | M16   | 551  | GLU  | C-N-CA     | 8.40  | 137.82      | 121.18   |
| 1   | R16   | 1380 | LYS  | O-C-N      | -8.40 | 113.22      | 122.12   |
| 18  | B     | 1811 | PRO  | O-C-N      | -8.40 | 113.02      | 123.10   |
| 10  | C32   | 1032 | THR  | O-C-N      | -8.39 | 110.79      | 122.37   |
| 18  | B     | 676  | ASP  | O-C-N      | -8.39 | 112.40      | 122.22   |
| 10  | C24   | 734  | LEU  | CA-C-N     | 8.39  | 128.88      | 119.32   |
| 10  | C24   | 734  | LEU  | C-N-CA     | 8.39  | 128.88      | 119.32   |
| 4   | T     | 160  | HIS  | CG-ND1-CE1 | 8.38  | 123.55      | 109.30   |
| 18  | B     | 298  | THR  | O-C-N      | -8.38 | 111.44      | 122.59   |
| 9   | K     | 891  | GLU  | CA-C-N     | 8.38  | 137.54      | 121.54   |
| 9   | K     | 891  | GLU  | C-N-CA     | 8.38  | 137.54      | 121.54   |
| 9   | K8    | 1215 | GLY  | CA-C-N     | 8.38  | 128.35      | 119.05   |
| 9   | K8    | 1215 | GLY  | C-N-CA     | 8.38  | 128.35      | 119.05   |
| 11  | A40   | 466  | SER  | CA-C-N     | -8.38 | 108.22      | 120.28   |
| 11  | A40   | 466  | SER  | C-N-CA     | -8.38 | 108.22      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 1120 | THR  | CA-C-N | 8.37  | 137.53      | 121.54   |
| 18  | B     | 1120 | THR  | C-N-CA | 8.37  | 137.53      | 121.54   |
| 2   | M8    | 551  | GLU  | CA-C-N | 8.37  | 137.75      | 121.18   |
| 2   | M8    | 551  | GLU  | C-N-CA | 8.37  | 137.75      | 121.18   |
| 12  | A48   | 466  | SER  | CA-C-N | -8.37 | 108.23      | 120.28   |
| 12  | A48   | 466  | SER  | C-N-CA | -8.37 | 108.23      | 120.28   |
| 1   | R     | 1380 | LYS  | O-C-N  | -8.36 | 113.26      | 122.12   |
| 9   | K     | 1215 | GLY  | CA-C-N | 8.36  | 128.33      | 119.05   |
| 9   | K     | 1215 | GLY  | C-N-CA | 8.36  | 128.33      | 119.05   |
| 10  | C32   | 1777 | SER  | O-C-N  | -8.36 | 110.93      | 122.46   |
| 2   | M     | 332  | MET  | CA-C-N | -8.35 | 109.09      | 120.28   |
| 2   | M     | 332  | MET  | C-N-CA | -8.35 | 109.09      | 120.28   |
| 2   | M     | 551  | GLU  | CA-C-N | 8.35  | 137.71      | 121.18   |
| 2   | M     | 551  | GLU  | C-N-CA | 8.35  | 137.71      | 121.18   |
| 11  | A24   | 466  | SER  | CA-C-N | -8.35 | 108.26      | 120.28   |
| 11  | A24   | 466  | SER  | C-N-CA | -8.35 | 108.26      | 120.28   |
| 10  | C32   | 1058 | GLU  | O-C-N  | -8.35 | 111.49      | 122.59   |
| 9   | K8    | 601  | VAL  | O-C-N  | -8.34 | 112.14      | 122.57   |
| 12  | A     | 466  | SER  | CA-C-N | -8.34 | 108.27      | 120.28   |
| 12  | A     | 466  | SER  | C-N-CA | -8.34 | 108.27      | 120.28   |
| 18  | B8    | 1120 | THR  | CA-C-N | 8.33  | 137.45      | 121.54   |
| 18  | B8    | 1120 | THR  | C-N-CA | 8.33  | 137.45      | 121.54   |
| 1   | R8    | 1380 | LYS  | O-C-N  | -8.33 | 113.29      | 122.12   |
| 10  | C     | 1058 | GLU  | O-C-N  | -8.33 | 111.51      | 122.59   |
| 10  | C32   | 734  | LEU  | CA-C-N | 8.32  | 128.81      | 119.32   |
| 10  | C32   | 734  | LEU  | C-N-CA | 8.32  | 128.81      | 119.32   |
| 2   | M16   | 332  | MET  | CA-C-N | -8.32 | 109.13      | 120.28   |
| 2   | M16   | 332  | MET  | C-N-CA | -8.32 | 109.13      | 120.28   |
| 10  | C16   | 1777 | SER  | O-C-N  | -8.32 | 110.98      | 122.46   |
| 14  | W     | 593  | GLY  | CA-C-N | 8.32  | 128.64      | 119.90   |
| 14  | W     | 593  | GLY  | C-N-CA | 8.32  | 128.64      | 119.90   |
| 11  | A16   | 466  | SER  | CA-C-N | -8.32 | 108.30      | 120.28   |
| 11  | A16   | 466  | SER  | C-N-CA | -8.32 | 108.30      | 120.28   |
| 2   | M8    | 332  | MET  | CA-C-N | -8.31 | 109.15      | 120.28   |
| 2   | M8    | 332  | MET  | C-N-CA | -8.31 | 109.15      | 120.28   |
| 7   | Q     | 277  | ASN  | CA-C-N | -8.31 | 111.45      | 119.76   |
| 7   | Q     | 277  | ASN  | C-N-CA | -8.31 | 111.45      | 119.76   |
| 10  | C24   | 1058 | GLU  | O-C-N  | -8.30 | 111.55      | 122.59   |
| 7   | Q8    | 275  | ILE  | O-C-N  | -8.30 | 112.19      | 122.57   |
| 10  | C8    | 1058 | GLU  | O-C-N  | -8.30 | 111.55      | 122.59   |
| 7   | Q8    | 277  | ASN  | CA-C-N | -8.30 | 111.46      | 119.76   |
| 7   | Q8    | 277  | ASN  | C-N-CA | -8.30 | 111.46      | 119.76   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 20  | E8    | 417  | LYS  | O-C-N  | -8.30 | 110.67      | 122.29   |
| 9   | K     | 1119 | ASN  | CA-C-N | 8.30  | 137.67      | 121.41   |
| 9   | K     | 1119 | ASN  | C-N-CA | 8.30  | 137.67      | 121.41   |
| 11  | A32   | 466  | SER  | CA-C-N | -8.29 | 108.34      | 120.28   |
| 11  | A32   | 466  | SER  | C-N-CA | -8.29 | 108.34      | 120.28   |
| 7   | Q8    | 220  | ASN  | CA-C-N | -8.29 | 108.86      | 122.54   |
| 7   | Q8    | 220  | ASN  | C-N-CA | -8.29 | 108.86      | 122.54   |
| 7   | Q16   | 275  | ILE  | O-C-N  | -8.29 | 112.20      | 122.57   |
| 10  | C24   | 1777 | SER  | O-C-N  | -8.29 | 111.02      | 122.46   |
| 1   | R8    | 1325 | GLN  | O-C-N  | -8.29 | 112.70      | 122.15   |
| 9   | K8    | 1089 | LYS  | O-C-N  | -8.28 | 111.58      | 122.59   |
| 10  | C16   | 1058 | GLU  | O-C-N  | -8.28 | 111.58      | 122.59   |
| 1   | R16   | 1325 | GLN  | O-C-N  | -8.27 | 112.72      | 122.15   |
| 7   | Q     | 275  | ILE  | O-C-N  | -8.27 | 112.23      | 122.57   |
| 19  | 4     | 343  | LEU  | O-C-N  | 8.27  | 129.20      | 120.85   |
| 10  | C     | 1777 | SER  | O-C-N  | -8.27 | 111.05      | 122.46   |
| 9   | K8    | 1119 | ASN  | CA-C-N | 8.27  | 137.61      | 121.41   |
| 9   | K8    | 1119 | ASN  | C-N-CA | 8.27  | 137.61      | 121.41   |
| 9   | K     | 601  | VAL  | O-C-N  | -8.26 | 112.24      | 122.57   |
| 20  | E     | 417  | LYS  | O-C-N  | -8.26 | 110.72      | 122.29   |
| 1   | R     | 1325 | GLN  | O-C-N  | -8.26 | 112.73      | 122.15   |
| 10  | C8    | 1777 | SER  | O-C-N  | -8.26 | 111.07      | 122.46   |
| 6   | O8    | 94   | GLY  | O-C-N  | -8.25 | 111.97      | 122.70   |
| 6   | O     | 94   | GLY  | O-C-N  | -8.25 | 111.97      | 122.70   |
| 6   | O16   | 94   | GLY  | O-C-N  | -8.24 | 111.99      | 122.70   |
| 10  | C     | 399  | HIS  | CA-C-N | 8.23  | 128.19      | 119.05   |
| 10  | C     | 399  | HIS  | C-N-CA | 8.23  | 128.19      | 119.05   |
| 2   | M     | 758  | GLU  | O-C-N  | -8.23 | 111.65      | 122.59   |
| 10  | C16   | 399  | HIS  | CA-C-N | 8.23  | 128.18      | 119.05   |
| 10  | C16   | 399  | HIS  | C-N-CA | 8.23  | 128.18      | 119.05   |
| 18  | B8    | 913  | SER  | CA-C-N | -8.23 | 109.96      | 123.04   |
| 18  | B8    | 913  | SER  | C-N-CA | -8.23 | 109.96      | 123.04   |
| 19  | 48    | 343  | LEU  | O-C-N  | 8.23  | 129.16      | 120.85   |
| 7   | Q     | 220  | ASN  | CA-C-N | -8.22 | 108.97      | 122.54   |
| 7   | Q     | 220  | ASN  | C-N-CA | -8.22 | 108.97      | 122.54   |
| 7   | Q16   | 220  | ASN  | CA-C-N | -8.22 | 108.97      | 122.54   |
| 7   | Q16   | 220  | ASN  | C-N-CA | -8.22 | 108.97      | 122.54   |
| 10  | C16   | 515  | ASP  | O-C-N  | 8.22  | 130.84      | 122.12   |
| 18  | B     | 1110 | LEU  | O-C-N  | -8.22 | 110.43      | 122.43   |
| 9   | K     | 1089 | LYS  | O-C-N  | -8.22 | 111.66      | 122.59   |
| 10  | C32   | 399  | HIS  | CA-C-N | 8.22  | 128.17      | 119.05   |
| 10  | C32   | 399  | HIS  | C-N-CA | 8.22  | 128.17      | 119.05   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 12  | A48   | 462  | THR  | O-C-N  | -8.22 | 111.66      | 122.59   |
| 18  | B     | 913  | SER  | CA-C-N | -8.21 | 109.99      | 123.04   |
| 18  | B     | 913  | SER  | C-N-CA | -8.21 | 109.99      | 123.04   |
| 2   | M     | 337  | ASP  | O-C-N  | -8.21 | 113.50      | 122.03   |
| 2   | M16   | 337  | ASP  | O-C-N  | -8.21 | 113.49      | 122.03   |
| 10  | C     | 454  | SER  | O-C-N  | -8.21 | 113.87      | 123.22   |
| 7   | Q16   | 277  | ASN  | CA-C-N | -8.20 | 111.56      | 119.76   |
| 7   | Q16   | 277  | ASN  | C-N-CA | -8.20 | 111.56      | 119.76   |
| 10  | C16   | 1788 | HIS  | O-C-N  | -8.20 | 110.23      | 122.28   |
| 10  | C8    | 399  | HIS  | CA-C-N | 8.20  | 128.15      | 119.05   |
| 10  | C8    | 399  | HIS  | C-N-CA | 8.20  | 128.15      | 119.05   |
| 14  | W     | 603  | LEU  | CA-C-N | 8.19  | 130.08      | 119.84   |
| 14  | W     | 603  | LEU  | C-N-CA | 8.19  | 130.08      | 119.84   |
| 10  | C8    | 454  | SER  | O-C-N  | -8.19 | 113.89      | 123.22   |
| 6   | O     | 179  | LYS  | O-C-N  | -8.18 | 113.72      | 123.13   |
| 11  | A24   | 462  | THR  | O-C-N  | -8.18 | 111.71      | 122.59   |
| 10  | C32   | 1781 | GLY  | CA-C-N | -8.18 | 109.46      | 121.24   |
| 10  | C32   | 1781 | GLY  | C-N-CA | -8.18 | 109.46      | 121.24   |
| 10  | C16   | 454  | SER  | O-C-N  | -8.18 | 113.90      | 123.22   |
| 17  | F     | 56   | PRO  | O-C-N  | 8.18  | 124.99      | 121.15   |
| 6   | O8    | 179  | LYS  | O-C-N  | -8.17 | 113.73      | 123.13   |
| 10  | C16   | 1781 | GLY  | CA-C-N | -8.17 | 109.47      | 121.24   |
| 10  | C16   | 1781 | GLY  | C-N-CA | -8.17 | 109.47      | 121.24   |
| 12  | A     | 462  | THR  | O-C-N  | -8.17 | 111.72      | 122.59   |
| 11  | A32   | 462  | THR  | O-C-N  | -8.17 | 111.72      | 122.59   |
| 6   | O16   | 179  | LYS  | O-C-N  | -8.17 | 113.74      | 123.13   |
| 10  | C     | 1788 | HIS  | O-C-N  | -8.17 | 110.27      | 122.28   |
| 2   | M8    | 337  | ASP  | O-C-N  | -8.17 | 113.54      | 122.03   |
| 10  | C24   | 399  | HIS  | CA-C-N | 8.17  | 128.12      | 119.05   |
| 10  | C24   | 399  | HIS  | C-N-CA | 8.17  | 128.12      | 119.05   |
| 18  | B8    | 1110 | LEU  | O-C-N  | -8.17 | 110.51      | 122.43   |
| 2   | M8    | 758  | GLU  | O-C-N  | -8.16 | 111.73      | 122.59   |
| 11  | A40   | 462  | THR  | O-C-N  | -8.16 | 111.73      | 122.59   |
| 10  | C8    | 1781 | GLY  | CA-C-N | -8.16 | 109.49      | 121.24   |
| 10  | C8    | 1781 | GLY  | C-N-CA | -8.16 | 109.49      | 121.24   |
| 9   | K8    | 1058 | GLU  | O-C-N  | -8.16 | 112.24      | 122.27   |
| 10  | C32   | 515  | ASP  | O-C-N  | 8.16  | 130.77      | 122.12   |
| 10  | C24   | 1788 | HIS  | O-C-N  | -8.16 | 110.29      | 122.28   |
| 9   | K8    | 1224 | GLY  | CA-C-N | 8.15  | 133.08      | 121.42   |
| 9   | K8    | 1224 | GLY  | C-N-CA | 8.15  | 133.08      | 121.42   |
| 18  | B     | 1961 | TYR  | O-C-N  | 8.15  | 128.78      | 121.36   |
| 10  | C32   | 1788 | HIS  | O-C-N  | -8.15 | 110.30      | 122.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 1051 | GLU  | CA-C-N | -8.14 | 105.98      | 121.54   |
| 9   | K     | 1051 | GLU  | C-N-CA | -8.14 | 105.98      | 121.54   |
| 9   | K     | 1269 | CYS  | O-C-N  | -8.14 | 111.64      | 122.23   |
| 11  | A32   | 28   | SER  | O-C-N  | -8.14 | 113.77      | 123.13   |
| 20  | E8    | 444  | VAL  | O-C-N  | -8.14 | 112.39      | 122.57   |
| 10  | C     | 515  | ASP  | O-C-N  | 8.14  | 130.75      | 122.12   |
| 11  | A16   | 462  | THR  | O-C-N  | -8.14 | 111.76      | 122.59   |
| 18  | B     | 985  | ASP  | CA-C-N | -8.14 | 109.42      | 120.90   |
| 18  | B     | 985  | ASP  | C-N-CA | -8.14 | 109.42      | 120.90   |
| 9   | K8    | 1269 | CYS  | O-C-N  | -8.14 | 111.65      | 122.23   |
| 18  | B     | 608  | SER  | CA-C-N | -8.14 | 105.99      | 121.54   |
| 18  | B     | 608  | SER  | C-N-CA | -8.14 | 105.99      | 121.54   |
| 18  | B8    | 1961 | TYR  | O-C-N  | 8.14  | 128.76      | 121.36   |
| 10  | C32   | 454  | SER  | O-C-N  | -8.14 | 113.94      | 123.22   |
| 10  | C24   | 1781 | GLY  | CA-C-N | -8.13 | 109.53      | 121.24   |
| 10  | C24   | 1781 | GLY  | C-N-CA | -8.13 | 109.53      | 121.24   |
| 9   | K     | 1224 | GLY  | CA-C-N | 8.13  | 133.05      | 121.42   |
| 9   | K     | 1224 | GLY  | C-N-CA | 8.13  | 133.05      | 121.42   |
| 10  | C     | 1781 | GLY  | CA-C-N | -8.13 | 109.53      | 121.24   |
| 10  | C     | 1781 | GLY  | C-N-CA | -8.13 | 109.53      | 121.24   |
| 18  | B8    | 608  | SER  | CA-C-N | -8.13 | 106.01      | 121.54   |
| 18  | B8    | 608  | SER  | C-N-CA | -8.13 | 106.01      | 121.54   |
| 2   | M16   | 758  | GLU  | O-C-N  | -8.12 | 111.78      | 122.59   |
| 10  | C8    | 1788 | HIS  | O-C-N  | -8.12 | 110.35      | 122.28   |
| 11  | A16   | 28   | SER  | O-C-N  | -8.12 | 113.79      | 123.13   |
| 18  | B     | 683  | ASN  | O-C-N  | -8.12 | 111.79      | 122.59   |
| 10  | C     | 105  | TRP  | O-C-N  | -8.12 | 111.98      | 122.20   |
| 17  | F16   | 56   | PRO  | O-C-N  | 8.11  | 124.96      | 121.15   |
| 20  | E     | 444  | VAL  | O-C-N  | -8.11 | 112.43      | 122.57   |
| 9   | K8    | 1051 | GLU  | CA-C-N | -8.11 | 106.05      | 121.54   |
| 9   | K8    | 1051 | GLU  | C-N-CA | -8.11 | 106.05      | 121.54   |
| 10  | C24   | 105  | TRP  | O-C-N  | -8.11 | 111.98      | 122.20   |
| 11  | A24   | 28   | SER  | O-C-N  | -8.10 | 113.81      | 123.13   |
| 10  | C8    | 515  | ASP  | O-C-N  | 8.10  | 130.71      | 122.12   |
| 18  | B8    | 985  | ASP  | CA-C-N | -8.10 | 109.47      | 120.90   |
| 18  | B8    | 985  | ASP  | C-N-CA | -8.10 | 109.47      | 120.90   |
| 5   | P16   | 685  | PRO  | O-C-N  | -8.10 | 114.44      | 123.03   |
| 18  | B     | 1477 | GLY  | O-C-N  | -8.10 | 112.17      | 122.70   |
| 18  | B     | 1707 | TRP  | O-C-N  | -8.10 | 113.73      | 122.07   |
| 18  | B8    | 1066 | ASP  | CA-C-N | -8.10 | 108.38      | 121.26   |
| 18  | B8    | 1066 | ASP  | C-N-CA | -8.10 | 108.38      | 121.26   |
| 18  | B8    | 1477 | GLY  | O-C-N  | -8.09 | 112.19      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 1235 | GLU  | O-C-N  | -8.08 | 111.84      | 122.59   |
| 10  | C32   | 105  | TRP  | O-C-N  | -8.08 | 112.01      | 122.20   |
| 18  | B     | 682  | TYR  | CA-C-N | -8.08 | 106.11      | 121.54   |
| 18  | B     | 682  | TYR  | C-N-CA | -8.08 | 106.11      | 121.54   |
| 10  | C8    | 105  | TRP  | O-C-N  | -8.08 | 112.02      | 122.20   |
| 18  | B8    | 682  | TYR  | CA-C-N | -8.07 | 106.12      | 121.54   |
| 18  | B8    | 682  | TYR  | C-N-CA | -8.07 | 106.12      | 121.54   |
| 11  | A40   | 28   | SER  | O-C-N  | -8.07 | 113.85      | 123.13   |
| 9   | K     | 1058 | GLU  | O-C-N  | -8.07 | 112.35      | 122.27   |
| 19  | 4     | 64   | ASP  | CA-C-N | 8.07  | 136.95      | 121.54   |
| 19  | 4     | 64   | ASP  | C-N-CA | 8.07  | 136.95      | 121.54   |
| 18  | B8    | 1279 | THR  | O-C-N  | -8.06 | 111.86      | 122.59   |
| 18  | B     | 1279 | THR  | O-C-N  | -8.06 | 111.87      | 122.59   |
| 10  | C24   | 454  | SER  | O-C-N  | -8.06 | 114.03      | 123.22   |
| 23  | J32   | 733  | ALA  | CA-C-N | 8.06  | 129.91      | 119.84   |
| 23  | J32   | 733  | ALA  | C-N-CA | 8.06  | 129.91      | 119.84   |
| 10  | C24   | 454  | SER  | CA-C-N | 8.05  | 132.87      | 122.00   |
| 10  | C24   | 454  | SER  | C-N-CA | 8.05  | 132.87      | 122.00   |
| 17  | F8    | 56   | PRO  | O-C-N  | 8.05  | 124.94      | 121.15   |
| 19  | 48    | 64   | ASP  | CA-C-N | 8.05  | 136.93      | 121.54   |
| 19  | 48    | 64   | ASP  | C-N-CA | 8.05  | 136.93      | 121.54   |
| 18  | B8    | 683  | ASN  | O-C-N  | -8.05 | 111.88      | 122.59   |
| 9   | K8    | 1235 | GLU  | O-C-N  | -8.05 | 111.88      | 122.59   |
| 10  | C16   | 105  | TRP  | O-C-N  | -8.05 | 112.06      | 122.20   |
| 10  | C24   | 515  | ASP  | O-C-N  | 8.05  | 130.65      | 122.12   |
| 23  | J16   | 733  | ALA  | CA-C-N | 8.05  | 129.90      | 119.84   |
| 23  | J16   | 733  | ALA  | C-N-CA | 8.05  | 129.90      | 119.84   |
| 18  | B8    | 1707 | TRP  | O-C-N  | -8.04 | 113.78      | 122.07   |
| 2   | M     | 527  | GLY  | O-C-N  | -8.04 | 112.25      | 122.70   |
| 18  | B8    | 1670 | SER  | O-C-N  | -8.04 | 112.32      | 123.01   |
| 10  | C16   | 631  | ASP  | O-C-N  | -8.04 | 111.90      | 122.59   |
| 20  | E     | 351  | SER  | O-C-N  | -8.04 | 111.90      | 122.59   |
| 2   | M8    | 761  | PRO  | CA-C-N | 8.03  | 136.87      | 121.54   |
| 2   | M8    | 761  | PRO  | C-N-CA | 8.03  | 136.87      | 121.54   |
| 1   | R16   | 1186 | THR  | O-C-N  | -8.03 | 111.92      | 122.59   |
| 10  | C24   | 626  | GLN  | CA-C-N | -8.03 | 107.52      | 121.97   |
| 10  | C24   | 626  | GLN  | C-N-CA | -8.03 | 107.52      | 121.97   |
| 1   | R8    | 1186 | THR  | O-C-N  | -8.02 | 111.92      | 122.59   |
| 23  | J24   | 733  | ALA  | CA-C-N | 8.02  | 129.87      | 119.84   |
| 23  | J24   | 733  | ALA  | C-N-CA | 8.02  | 129.87      | 119.84   |
| 1   | R     | 1186 | THR  | O-C-N  | -8.02 | 111.92      | 122.59   |
| 20  | E     | 419  | ASN  | O-C-N  | -8.02 | 111.92      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | N16   | 45   | GLY  | O-C-N  | -8.02 | 117.42      | 123.35   |
| 10  | C     | 631  | ASP  | O-C-N  | -8.02 | 111.93      | 122.59   |
| 1   | R     | 1248 | PRO  | O-C-N  | -8.01 | 113.48      | 123.10   |
| 2   | M     | 761  | PRO  | CA-C-N | 8.01  | 136.85      | 121.54   |
| 2   | M     | 761  | PRO  | C-N-CA | 8.01  | 136.85      | 121.54   |
| 5   | P     | 685  | PRO  | O-C-N  | -8.01 | 114.54      | 123.03   |
| 10  | C     | 420  | TYR  | O-C-N  | -8.01 | 111.70      | 122.43   |
| 10  | C     | 626  | GLN  | CA-C-N | -8.01 | 107.55      | 121.97   |
| 10  | C     | 626  | GLN  | C-N-CA | -8.01 | 107.55      | 121.97   |
| 20  | E8    | 351  | SER  | O-C-N  | -8.01 | 111.94      | 122.59   |
| 1   | R16   | 1238 | GLY  | O-C-N  | -8.01 | 112.29      | 122.70   |
| 20  | E8    | 419  | ASN  | O-C-N  | -8.01 | 111.94      | 122.59   |
| 23  | J8    | 733  | ALA  | CA-C-N | 8.01  | 129.85      | 119.84   |
| 23  | J8    | 733  | ALA  | C-N-CA | 8.01  | 129.85      | 119.84   |
| 10  | C32   | 1542 | PHE  | CA-C-N | 8.01  | 136.84      | 121.54   |
| 10  | C32   | 1542 | PHE  | C-N-CA | 8.01  | 136.84      | 121.54   |
| 10  | C16   | 420  | TYR  | O-C-N  | -8.00 | 111.71      | 122.43   |
| 18  | B     | 1670 | SER  | O-C-N  | -8.00 | 112.37      | 123.01   |
| 10  | C24   | 631  | ASP  | O-C-N  | -8.00 | 111.95      | 122.59   |
| 18  | B     | 684  | ILE  | CA-C-N | -8.00 | 106.26      | 121.54   |
| 18  | B     | 684  | ILE  | C-N-CA | -8.00 | 106.26      | 121.54   |
| 10  | C32   | 420  | TYR  | O-C-N  | -8.00 | 111.71      | 122.43   |
| 2   | M8    | 527  | GLY  | O-C-N  | -8.00 | 112.31      | 122.70   |
| 10  | C8    | 420  | TYR  | O-C-N  | -7.99 | 111.72      | 122.43   |
| 2   | M16   | 761  | PRO  | CA-C-N | 7.99  | 136.80      | 121.54   |
| 2   | M16   | 761  | PRO  | C-N-CA | 7.99  | 136.80      | 121.54   |
| 9   | K8    | 1055 | THR  | CA-C-N | -7.99 | 107.59      | 121.97   |
| 9   | K8    | 1055 | THR  | C-N-CA | -7.99 | 107.59      | 121.97   |
| 10  | C8    | 1542 | PHE  | CA-C-N | 7.99  | 136.80      | 121.54   |
| 10  | C8    | 1542 | PHE  | C-N-CA | 7.99  | 136.80      | 121.54   |
| 10  | C16   | 626  | GLN  | CA-C-N | -7.99 | 107.60      | 121.97   |
| 10  | C16   | 626  | GLN  | C-N-CA | -7.99 | 107.60      | 121.97   |
| 10  | C32   | 626  | GLN  | CA-C-N | -7.99 | 107.60      | 121.97   |
| 10  | C32   | 626  | GLN  | C-N-CA | -7.99 | 107.60      | 121.97   |
| 9   | K     | 1055 | THR  | CA-C-N | -7.98 | 107.60      | 121.97   |
| 9   | K     | 1055 | THR  | C-N-CA | -7.98 | 107.60      | 121.97   |
| 10  | C24   | 420  | TYR  | O-C-N  | -7.98 | 111.74      | 122.43   |
| 18  | B8    | 684  | ILE  | CA-C-N | -7.98 | 106.30      | 121.54   |
| 18  | B8    | 684  | ILE  | C-N-CA | -7.98 | 106.30      | 121.54   |
| 17  | F24   | 56   | PRO  | O-C-N  | 7.98  | 124.90      | 121.15   |
| 10  | C24   | 1542 | PHE  | CA-C-N | 7.98  | 136.78      | 121.54   |
| 10  | C24   | 1542 | PHE  | C-N-CA | 7.98  | 136.78      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 631  | ASP  | O-C-N  | -7.97 | 111.99      | 122.59   |
| 2   | M16   | 527  | GLY  | O-C-N  | -7.97 | 112.34      | 122.70   |
| 9   | K     | 1061 | GLY  | CA-C-N | 7.97  | 129.80      | 119.84   |
| 9   | K     | 1061 | GLY  | C-N-CA | 7.97  | 129.80      | 119.84   |
| 9   | K8    | 1061 | GLY  | CA-C-N | 7.97  | 129.80      | 119.84   |
| 9   | K8    | 1061 | GLY  | C-N-CA | 7.97  | 129.80      | 119.84   |
| 1   | R16   | 1248 | PRO  | O-C-N  | -7.96 | 113.54      | 123.10   |
| 18  | B8    | 384  | ASP  | O-C-N  | -7.96 | 111.87      | 122.38   |
| 5   | P8    | 685  | PRO  | O-C-N  | -7.96 | 114.59      | 123.03   |
| 1   | R8    | 1248 | PRO  | O-C-N  | -7.96 | 113.55      | 123.10   |
| 3   | N8    | 45   | GLY  | O-C-N  | -7.95 | 117.47      | 123.35   |
| 10  | C16   | 1542 | PHE  | CA-C-N | 7.95  | 136.72      | 121.54   |
| 10  | C16   | 1542 | PHE  | C-N-CA | 7.95  | 136.72      | 121.54   |
| 18  | B8    | 1748 | HIS  | O-C-N  | -7.95 | 113.05      | 122.27   |
| 12  | A48   | 737  | GLU  | O-C-N  | -7.95 | 113.23      | 123.32   |
| 10  | C16   | 628  | GLY  | CA-C-N | 7.94  | 136.71      | 121.54   |
| 10  | C16   | 628  | GLY  | C-N-CA | 7.94  | 136.71      | 121.54   |
| 18  | B     | 384  | ASP  | O-C-N  | -7.94 | 111.90      | 122.38   |
| 10  | C32   | 1772 | ASP  | O-C-N  | -7.94 | 111.93      | 122.57   |
| 11  | A40   | 737  | GLU  | O-C-N  | -7.93 | 113.24      | 123.32   |
| 10  | C     | 1772 | ASP  | O-C-N  | -7.93 | 111.94      | 122.57   |
| 11  | A16   | 737  | GLU  | O-C-N  | -7.93 | 113.25      | 123.32   |
| 20  | E     | 427  | MET  | CA-C-N | -7.93 | 109.42      | 121.87   |
| 20  | E     | 427  | MET  | C-N-CA | -7.93 | 109.42      | 121.87   |
| 10  | C     | 1336 | ALA  | O-C-N  | -7.92 | 112.05      | 122.59   |
| 10  | C32   | 628  | GLY  | CA-C-N | 7.92  | 136.67      | 121.54   |
| 10  | C32   | 628  | GLY  | C-N-CA | 7.92  | 136.67      | 121.54   |
| 2   | M     | 336  | SER  | CA-C-N | -7.92 | 110.20      | 120.65   |
| 2   | M     | 336  | SER  | C-N-CA | -7.92 | 110.20      | 120.65   |
| 9   | K     | 1057 | GLU  | O-C-N  | -7.92 | 112.06      | 122.59   |
| 20  | E8    | 427  | MET  | CA-C-N | -7.92 | 109.44      | 121.87   |
| 20  | E8    | 427  | MET  | C-N-CA | -7.92 | 109.44      | 121.87   |
| 11  | A24   | 737  | GLU  | O-C-N  | -7.91 | 113.27      | 123.32   |
| 10  | C     | 628  | GLY  | CA-C-N | 7.91  | 136.65      | 121.54   |
| 10  | C     | 628  | GLY  | C-N-CA | 7.91  | 136.65      | 121.54   |
| 10  | C24   | 1336 | ALA  | O-C-N  | -7.91 | 112.07      | 122.59   |
| 10  | C8    | 1772 | ASP  | O-C-N  | -7.91 | 111.97      | 122.57   |
| 18  | B     | 1748 | HIS  | O-C-N  | -7.91 | 113.09      | 122.27   |
| 18  | B     | 1067 | SER  | O-C-N  | -7.91 | 112.50      | 123.01   |
| 11  | A32   | 737  | GLU  | O-C-N  | -7.90 | 113.28      | 123.32   |
| 9   | K     | 1251 | HIS  | CA-C-N | 7.90  | 131.20      | 120.38   |
| 9   | K     | 1251 | HIS  | C-N-CA | 7.90  | 131.20      | 120.38   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K8    | 1057 | GLU  | O-C-N  | -7.89 | 112.09      | 122.59   |
| 18  | B     | 1808 | GLY  | CA-C-N | 7.89  | 134.00      | 122.16   |
| 18  | B     | 1808 | GLY  | C-N-CA | 7.89  | 134.00      | 122.16   |
| 10  | C24   | 628  | GLY  | CA-C-N | 7.89  | 136.61      | 121.54   |
| 10  | C24   | 628  | GLY  | C-N-CA | 7.89  | 136.61      | 121.54   |
| 12  | A     | 737  | GLU  | O-C-N  | -7.89 | 113.30      | 123.32   |
| 10  | C     | 675  | ASP  | CA-C-N | 7.88  | 137.71      | 121.94   |
| 10  | C     | 675  | ASP  | C-N-CA | 7.88  | 137.71      | 121.94   |
| 18  | B8    | 1883 | TYR  | CA-C-N | 7.88  | 130.84      | 120.28   |
| 18  | B8    | 1883 | TYR  | C-N-CA | 7.88  | 130.84      | 120.28   |
| 9   | K8    | 1284 | MET  | O-C-N  | -7.88 | 109.73      | 122.42   |
| 18  | B8    | 971  | ASP  | O-C-N  | -7.88 | 112.11      | 122.59   |
| 1   | R8    | 1238 | GLY  | O-C-N  | -7.87 | 112.46      | 122.70   |
| 9   | K8    | 1251 | HIS  | CA-C-N | 7.87  | 131.16      | 120.38   |
| 9   | K8    | 1251 | HIS  | C-N-CA | 7.87  | 131.16      | 120.38   |
| 9   | K8    | 641  | THR  | CA-C-N | 7.87  | 136.57      | 121.54   |
| 9   | K8    | 641  | THR  | C-N-CA | 7.87  | 136.57      | 121.54   |
| 10  | C8    | 1336 | ALA  | O-C-N  | -7.87 | 112.12      | 122.59   |
| 2   | M8    | 336  | SER  | CA-C-N | -7.87 | 110.27      | 120.65   |
| 2   | M8    | 336  | SER  | C-N-CA | -7.87 | 110.27      | 120.65   |
| 10  | C24   | 675  | ASP  | CA-C-N | 7.87  | 137.67      | 121.94   |
| 10  | C24   | 675  | ASP  | C-N-CA | 7.87  | 137.67      | 121.94   |
| 10  | C24   | 1169 | ASN  | CA-C-N | 7.87  | 136.13      | 121.97   |
| 10  | C24   | 1169 | ASN  | C-N-CA | 7.87  | 136.13      | 121.97   |
| 10  | C16   | 1772 | ASP  | O-C-N  | -7.86 | 112.04      | 122.57   |
| 14  | W     | 594  | PRO  | CA-C-N | 7.86  | 131.13      | 120.44   |
| 14  | W     | 594  | PRO  | C-N-CA | 7.86  | 131.13      | 120.44   |
| 10  | C8    | 675  | ASP  | CA-C-N | 7.86  | 137.65      | 121.94   |
| 10  | C8    | 675  | ASP  | C-N-CA | 7.86  | 137.65      | 121.94   |
| 10  | C     | 625  | SER  | O-C-N  | -7.86 | 112.14      | 122.59   |
| 10  | C8    | 1169 | ASN  | CA-C-N | 7.85  | 136.11      | 121.97   |
| 10  | C8    | 1169 | ASN  | C-N-CA | 7.85  | 136.11      | 121.97   |
| 18  | B8    | 973  | ASP  | O-C-N  | -7.85 | 109.84      | 122.41   |
| 18  | B     | 121  | GLN  | O-C-N  | -7.85 | 113.55      | 122.03   |
| 18  | B     | 973  | ASP  | O-C-N  | -7.85 | 109.85      | 122.41   |
| 10  | C32   | 1336 | ALA  | O-C-N  | -7.85 | 112.15      | 122.59   |
| 18  | B8    | 1360 | SER  | CA-C-N | -7.85 | 108.97      | 120.28   |
| 18  | B8    | 1360 | SER  | C-N-CA | -7.85 | 108.97      | 120.28   |
| 10  | C     | 1169 | ASN  | CA-C-N | 7.85  | 136.10      | 121.97   |
| 10  | C     | 1169 | ASN  | C-N-CA | 7.85  | 136.10      | 121.97   |
| 19  | 48    | 66   | ALA  | O-C-N  | -7.85 | 112.16      | 122.59   |
| 9   | K     | 1284 | MET  | O-C-N  | -7.84 | 109.79      | 122.42   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | R     | 1238 | GLY  | O-C-N  | -7.84 | 112.50      | 122.70   |
| 3   | N     | 45   | GLY  | O-C-N  | -7.84 | 117.55      | 123.35   |
| 10  | C16   | 675  | ASP  | CA-C-N | 7.84  | 137.63      | 121.94   |
| 10  | C16   | 675  | ASP  | C-N-CA | 7.84  | 137.63      | 121.94   |
| 10  | C24   | 1772 | ASP  | O-C-N  | -7.84 | 112.06      | 122.57   |
| 18  | B     | 1360 | SER  | CA-C-N | -7.84 | 108.99      | 120.28   |
| 18  | B     | 1360 | SER  | C-N-CA | -7.84 | 108.99      | 120.28   |
| 18  | B8    | 1808 | GLY  | CA-C-N | 7.84  | 133.92      | 122.16   |
| 18  | B8    | 1808 | GLY  | C-N-CA | 7.84  | 133.92      | 122.16   |
| 18  | B8    | 1228 | SER  | CA-C-N | 7.84  | 136.77      | 121.41   |
| 18  | B8    | 1228 | SER  | C-N-CA | 7.84  | 136.77      | 121.41   |
| 10  | C16   | 1353 | ASP  | CA-C-N | 7.83  | 136.76      | 121.41   |
| 10  | C16   | 1353 | ASP  | C-N-CA | 7.83  | 136.76      | 121.41   |
| 10  | C     | 1083 | SER  | O-C-N  | -7.83 | 112.17      | 122.59   |
| 10  | C32   | 1353 | ASP  | CA-C-N | 7.83  | 136.76      | 121.41   |
| 10  | C32   | 1353 | ASP  | C-N-CA | 7.83  | 136.76      | 121.41   |
| 18  | B     | 1883 | TYR  | CA-C-N | 7.83  | 130.77      | 120.28   |
| 18  | B     | 1883 | TYR  | C-N-CA | 7.83  | 130.77      | 120.28   |
| 18  | B8    | 1073 | GLY  | CA-C-N | 7.83  | 130.77      | 120.28   |
| 18  | B8    | 1073 | GLY  | C-N-CA | 7.83  | 130.77      | 120.28   |
| 2   | M16   | 336  | SER  | CA-C-N | -7.83 | 110.32      | 120.65   |
| 2   | M16   | 336  | SER  | C-N-CA | -7.83 | 110.32      | 120.65   |
| 18  | B     | 1228 | SER  | CA-C-N | 7.83  | 136.75      | 121.41   |
| 18  | B     | 1228 | SER  | C-N-CA | 7.83  | 136.75      | 121.41   |
| 20  | E     | 341  | TYR  | CA-C-N | -7.82 | 106.60      | 121.54   |
| 20  | E     | 341  | TYR  | C-N-CA | -7.82 | 106.60      | 121.54   |
| 10  | C16   | 625  | SER  | O-C-N  | -7.82 | 112.19      | 122.59   |
| 10  | C16   | 1336 | ALA  | O-C-N  | -7.82 | 112.19      | 122.59   |
| 10  | C8    | 1353 | ASP  | CA-C-N | 7.82  | 136.73      | 121.41   |
| 10  | C8    | 1353 | ASP  | C-N-CA | 7.82  | 136.73      | 121.41   |
| 10  | C16   | 1169 | ASN  | CA-C-N | 7.82  | 136.04      | 121.97   |
| 10  | C16   | 1169 | ASN  | C-N-CA | 7.82  | 136.04      | 121.97   |
| 10  | C32   | 625  | SER  | O-C-N  | -7.82 | 112.20      | 122.59   |
| 18  | B     | 971  | ASP  | O-C-N  | -7.81 | 112.20      | 122.59   |
| 10  | C16   | 848  | CYS  | CA-C-N | -7.80 | 106.64      | 121.54   |
| 10  | C16   | 848  | CYS  | C-N-CA | -7.80 | 106.64      | 121.54   |
| 18  | B8    | 121  | GLN  | O-C-N  | -7.80 | 113.60      | 122.03   |
| 10  | C32   | 1169 | ASN  | CA-C-N | 7.80  | 136.01      | 121.97   |
| 10  | C32   | 1169 | ASN  | C-N-CA | 7.80  | 136.01      | 121.97   |
| 19  | 4     | 66   | ALA  | O-C-N  | -7.80 | 112.22      | 122.59   |
| 9   | K     | 641  | THR  | CA-C-N | 7.80  | 136.44      | 121.54   |
| 9   | K     | 641  | THR  | C-N-CA | 7.80  | 136.44      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 675  | ASP  | CA-C-N | 7.80  | 137.53      | 121.94   |
| 10  | C32   | 675  | ASP  | C-N-CA | 7.80  | 137.53      | 121.94   |
| 18  | B     | 687  | SER  | CA-C-N | -7.79 | 106.13      | 121.41   |
| 18  | B     | 687  | SER  | C-N-CA | -7.79 | 106.13      | 121.41   |
| 20  | E8    | 341  | TYR  | CA-C-N | -7.79 | 106.65      | 121.54   |
| 20  | E8    | 341  | TYR  | C-N-CA | -7.79 | 106.65      | 121.54   |
| 10  | C8    | 282  | LYS  | CA-C-N | 7.79  | 136.43      | 121.54   |
| 10  | C8    | 282  | LYS  | C-N-CA | 7.79  | 136.43      | 121.54   |
| 2   | M     | 348  | GLU  | O-C-N  | -7.79 | 112.23      | 122.59   |
| 2   | M16   | 348  | GLU  | O-C-N  | -7.79 | 112.23      | 122.59   |
| 10  | C24   | 1083 | SER  | O-C-N  | -7.79 | 112.23      | 122.59   |
| 10  | C16   | 1083 | SER  | O-C-N  | -7.79 | 112.23      | 122.59   |
| 18  | B     | 1073 | GLY  | CA-C-N | 7.79  | 130.71      | 120.28   |
| 18  | B     | 1073 | GLY  | C-N-CA | 7.79  | 130.71      | 120.28   |
| 10  | C24   | 1353 | ASP  | CA-C-N | 7.78  | 136.66      | 121.41   |
| 10  | C24   | 1353 | ASP  | C-N-CA | 7.78  | 136.66      | 121.41   |
| 18  | B8    | 687  | SER  | CA-C-N | -7.78 | 106.16      | 121.41   |
| 18  | B8    | 687  | SER  | C-N-CA | -7.78 | 106.16      | 121.41   |
| 1   | R8    | 1190 | VAL  | O-C-N  | -7.78 | 112.85      | 122.57   |
| 10  | C     | 1353 | ASP  | CA-C-N | 7.78  | 136.65      | 121.41   |
| 10  | C     | 1353 | ASP  | C-N-CA | 7.78  | 136.65      | 121.41   |
| 10  | C32   | 848  | CYS  | CA-C-N | -7.78 | 106.69      | 121.54   |
| 10  | C32   | 848  | CYS  | C-N-CA | -7.78 | 106.69      | 121.54   |
| 10  | C     | 848  | CYS  | CA-C-N | -7.77 | 106.69      | 121.54   |
| 10  | C     | 848  | CYS  | C-N-CA | -7.77 | 106.69      | 121.54   |
| 10  | C16   | 1784 | GLY  | O-C-N  | -7.77 | 113.40      | 122.34   |
| 10  | C8    | 671  | LYS  | O-C-N  | -7.77 | 111.57      | 122.76   |
| 10  | C32   | 1083 | SER  | O-C-N  | -7.77 | 112.25      | 122.59   |
| 2   | M8    | 348  | GLU  | O-C-N  | -7.77 | 112.26      | 122.59   |
| 10  | C24   | 671  | LYS  | O-C-N  | -7.77 | 111.58      | 122.76   |
| 18  | B     | 1788 | ILE  | O-C-N  | -7.77 | 112.86      | 122.57   |
| 10  | C     | 282  | LYS  | CA-C-N | 7.76  | 136.37      | 121.54   |
| 10  | C     | 282  | LYS  | C-N-CA | 7.76  | 136.37      | 121.54   |
| 18  | B     | 410  | GLN  | CA-C-N | 7.76  | 131.71      | 120.38   |
| 18  | B     | 410  | GLN  | C-N-CA | 7.76  | 131.71      | 120.38   |
| 18  | B     | 821  | PHE  | CA-C-N | -7.76 | 113.56      | 123.19   |
| 18  | B     | 821  | PHE  | C-N-CA | -7.76 | 113.56      | 123.19   |
| 18  | B8    | 821  | PHE  | CA-C-N | -7.76 | 113.57      | 123.19   |
| 18  | B8    | 821  | PHE  | C-N-CA | -7.76 | 113.57      | 123.19   |
| 18  | B8    | 1788 | ILE  | O-C-N  | -7.76 | 112.87      | 122.57   |
| 12  | A     | 556  | LYS  | CA-C-N | -7.76 | 109.54      | 121.02   |
| 12  | A     | 556  | LYS  | C-N-CA | -7.76 | 109.54      | 121.02   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 848  | CYS  | CA-C-N | -7.76 | 106.73      | 121.54   |
| 10  | C8    | 848  | CYS  | C-N-CA | -7.76 | 106.73      | 121.54   |
| 18  | B     | 1677 | ARG  | CA-C-N | -7.76 | 106.72      | 121.54   |
| 18  | B     | 1677 | ARG  | C-N-CA | -7.76 | 106.72      | 121.54   |
| 18  | B8    | 1677 | ARG  | CA-C-N | -7.76 | 106.72      | 121.54   |
| 18  | B8    | 1677 | ARG  | C-N-CA | -7.76 | 106.72      | 121.54   |
| 10  | C8    | 1083 | SER  | O-C-N  | -7.75 | 112.28      | 122.59   |
| 10  | C32   | 671  | LYS  | O-C-N  | -7.75 | 111.59      | 122.76   |
| 10  | C16   | 1056 | VAL  | CA-C-N | -7.75 | 109.47      | 121.56   |
| 10  | C16   | 1056 | VAL  | C-N-CA | -7.75 | 109.47      | 121.56   |
| 18  | B8    | 502  | ASP  | O-C-N  | -7.75 | 112.39      | 122.39   |
| 10  | C24   | 848  | CYS  | CA-C-N | -7.75 | 106.74      | 121.54   |
| 10  | C24   | 848  | CYS  | C-N-CA | -7.75 | 106.74      | 121.54   |
| 10  | C24   | 1075 | ASP  | CA-C-N | 7.75  | 136.34      | 121.54   |
| 10  | C24   | 1075 | ASP  | C-N-CA | 7.75  | 136.34      | 121.54   |
| 10  | C24   | 282  | LYS  | CA-C-N | 7.74  | 136.32      | 121.54   |
| 10  | C24   | 282  | LYS  | C-N-CA | 7.74  | 136.32      | 121.54   |
| 10  | C     | 671  | LYS  | O-C-N  | -7.74 | 111.61      | 122.76   |
| 18  | B8    | 410  | GLN  | CA-C-N | 7.74  | 131.68      | 120.38   |
| 18  | B8    | 410  | GLN  | C-N-CA | 7.74  | 131.68      | 120.38   |
| 5   | P8    | 147  | LEU  | O-C-N  | -7.73 | 114.58      | 121.31   |
| 10  | C32   | 1784 | GLY  | O-C-N  | -7.73 | 113.45      | 122.34   |
| 5   | P16   | 147  | LEU  | O-C-N  | -7.73 | 114.59      | 121.31   |
| 5   | P16   | 267  | ARG  | CA-C-N | 7.73  | 130.49      | 120.44   |
| 5   | P16   | 267  | ARG  | C-N-CA | 7.73  | 130.49      | 120.44   |
| 10  | C16   | 282  | LYS  | CA-C-N | 7.73  | 136.30      | 121.54   |
| 10  | C16   | 282  | LYS  | C-N-CA | 7.73  | 136.30      | 121.54   |
| 10  | C32   | 282  | LYS  | CA-C-N | 7.73  | 136.30      | 121.54   |
| 10  | C32   | 282  | LYS  | C-N-CA | 7.73  | 136.30      | 121.54   |
| 9   | K8    | 583  | GLU  | O-C-N  | 7.72  | 130.43      | 122.09   |
| 10  | C     | 253  | ASP  | CA-C-N | 7.72  | 130.63      | 120.28   |
| 10  | C     | 253  | ASP  | C-N-CA | 7.72  | 130.63      | 120.28   |
| 5   | P     | 267  | ARG  | CA-C-N | 7.72  | 130.48      | 120.44   |
| 5   | P     | 267  | ARG  | C-N-CA | 7.72  | 130.48      | 120.44   |
| 10  | C     | 1441 | TYR  | O-C-N  | -7.72 | 112.16      | 122.43   |
| 10  | C8    | 253  | ASP  | CA-C-N | 7.72  | 130.62      | 120.28   |
| 10  | C8    | 253  | ASP  | C-N-CA | 7.72  | 130.62      | 120.28   |
| 10  | C16   | 671  | LYS  | O-C-N  | -7.71 | 111.65      | 122.76   |
| 10  | C24   | 625  | SER  | O-C-N  | -7.71 | 112.33      | 122.59   |
| 18  | B     | 1601 | VAL  | CA-C-N | -7.71 | 106.81      | 121.54   |
| 18  | B     | 1601 | VAL  | C-N-CA | -7.71 | 106.81      | 121.54   |
| 18  | B     | 502  | ASP  | O-C-N  | -7.71 | 112.44      | 122.39   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | R16   | 1190 | VAL  | O-C-N  | -7.71 | 112.94      | 122.57   |
| 10  | C16   | 1075 | ASP  | CA-C-N | 7.71  | 136.26      | 121.54   |
| 10  | C16   | 1075 | ASP  | C-N-CA | 7.71  | 136.26      | 121.54   |
| 18  | B8    | 1601 | VAL  | CA-C-N | -7.70 | 106.83      | 121.54   |
| 18  | B8    | 1601 | VAL  | C-N-CA | -7.70 | 106.83      | 121.54   |
| 10  | C16   | 1441 | TYR  | O-C-N  | -7.70 | 112.19      | 122.43   |
| 10  | C24   | 1784 | GLY  | O-C-N  | -7.70 | 113.49      | 122.34   |
| 10  | C8    | 1784 | GLY  | O-C-N  | -7.70 | 113.49      | 122.34   |
| 10  | C32   | 1441 | TYR  | O-C-N  | -7.70 | 112.19      | 122.43   |
| 5   | P     | 147  | LEU  | O-C-N  | -7.69 | 114.62      | 121.31   |
| 10  | C32   | 1056 | VAL  | CA-C-N | -7.69 | 109.56      | 121.56   |
| 10  | C32   | 1056 | VAL  | C-N-CA | -7.69 | 109.56      | 121.56   |
| 9   | K8    | 1223 | ASP  | CA-C-N | 7.69  | 136.49      | 121.41   |
| 9   | K8    | 1223 | ASP  | C-N-CA | 7.69  | 136.49      | 121.41   |
| 12  | A48   | 556  | LYS  | CA-C-N | -7.69 | 109.63      | 121.02   |
| 12  | A48   | 556  | LYS  | C-N-CA | -7.69 | 109.63      | 121.02   |
| 10  | C8    | 1056 | VAL  | CA-C-N | -7.69 | 109.57      | 121.56   |
| 10  | C8    | 1056 | VAL  | C-N-CA | -7.69 | 109.57      | 121.56   |
| 5   | P8    | 267  | ARG  | CA-C-N | 7.69  | 130.43      | 120.44   |
| 5   | P8    | 267  | ARG  | C-N-CA | 7.69  | 130.43      | 120.44   |
| 10  | C24   | 1056 | VAL  | CA-C-N | -7.68 | 109.57      | 121.56   |
| 10  | C24   | 1056 | VAL  | C-N-CA | -7.68 | 109.57      | 121.56   |
| 18  | B8    | 1807 | PRO  | CA-C-N | -7.68 | 106.35      | 121.41   |
| 18  | B8    | 1807 | PRO  | C-N-CA | -7.68 | 106.35      | 121.41   |
| 5   | P     | 61   | ASP  | CA-C-N | -7.68 | 109.30      | 123.05   |
| 5   | P     | 61   | ASP  | C-N-CA | -7.68 | 109.30      | 123.05   |
| 11  | A24   | 556  | LYS  | CA-C-N | -7.68 | 109.65      | 121.02   |
| 11  | A24   | 556  | LYS  | C-N-CA | -7.68 | 109.65      | 121.02   |
| 10  | C32   | 1075 | ASP  | CA-C-N | 7.68  | 136.22      | 121.54   |
| 10  | C32   | 1075 | ASP  | C-N-CA | 7.68  | 136.22      | 121.54   |
| 10  | C24   | 1441 | TYR  | O-C-N  | -7.68 | 112.22      | 122.43   |
| 18  | B     | 1807 | PRO  | CA-C-N | -7.68 | 106.36      | 121.41   |
| 18  | B     | 1807 | PRO  | C-N-CA | -7.68 | 106.36      | 121.41   |
| 10  | C     | 439  | LEU  | CA-C-N | 7.68  | 128.07      | 119.32   |
| 10  | C     | 439  | LEU  | C-N-CA | 7.68  | 128.07      | 119.32   |
| 18  | B8    | 1067 | SER  | O-C-N  | -7.68 | 112.55      | 123.07   |
| 10  | C32   | 253  | ASP  | CA-C-N | 7.68  | 130.57      | 120.28   |
| 10  | C32   | 253  | ASP  | C-N-CA | 7.68  | 130.57      | 120.28   |
| 10  | C     | 1056 | VAL  | CA-C-N | -7.67 | 109.59      | 121.56   |
| 10  | C     | 1056 | VAL  | C-N-CA | -7.67 | 109.59      | 121.56   |
| 10  | C     | 1784 | GLY  | O-C-N  | -7.67 | 113.51      | 122.34   |
| 10  | C8    | 1075 | ASP  | CA-C-N | 7.67  | 136.20      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1075 | ASP  | C-N-CA | 7.67  | 136.20      | 121.54   |
| 11  | A16   | 556  | LYS  | CA-C-N | -7.67 | 109.67      | 121.02   |
| 11  | A16   | 556  | LYS  | C-N-CA | -7.67 | 109.67      | 121.02   |
| 1   | R     | 1190 | VAL  | O-C-N  | -7.67 | 112.98      | 122.57   |
| 9   | K     | 1223 | ASP  | CA-C-N | 7.67  | 136.44      | 121.41   |
| 9   | K     | 1223 | ASP  | C-N-CA | 7.67  | 136.44      | 121.41   |
| 15  | J     | 631  | GLU  | CA-C-N | 7.67  | 130.88      | 120.38   |
| 15  | J     | 631  | GLU  | C-N-CA | 7.67  | 130.88      | 120.38   |
| 10  | C32   | 464  | ASN  | O-C-N  | 7.67  | 130.25      | 122.12   |
| 10  | C16   | 253  | ASP  | CA-C-N | 7.67  | 130.55      | 120.28   |
| 10  | C16   | 253  | ASP  | C-N-CA | 7.67  | 130.55      | 120.28   |
| 5   | P16   | 61   | ASP  | CA-C-N | -7.67 | 109.33      | 123.05   |
| 5   | P16   | 61   | ASP  | C-N-CA | -7.67 | 109.33      | 123.05   |
| 7   | Q16   | 88   | ASN  | O-C-N  | -7.67 | 112.39      | 122.59   |
| 10  | C     | 1075 | ASP  | CA-C-N | 7.66  | 136.18      | 121.54   |
| 10  | C     | 1075 | ASP  | C-N-CA | 7.66  | 136.18      | 121.54   |
| 18  | B     | 1803 | THR  | CA-C-N | -7.66 | 106.91      | 121.54   |
| 18  | B     | 1803 | THR  | C-N-CA | -7.66 | 106.91      | 121.54   |
| 5   | P8    | 61   | ASP  | CA-C-N | -7.66 | 109.34      | 123.05   |
| 5   | P8    | 61   | ASP  | C-N-CA | -7.66 | 109.34      | 123.05   |
| 18  | B     | 1671 | ASP  | O-C-N  | -7.66 | 112.38      | 122.33   |
| 11  | A32   | 556  | LYS  | CA-C-N | -7.66 | 109.69      | 121.02   |
| 11  | A32   | 556  | LYS  | C-N-CA | -7.66 | 109.69      | 121.02   |
| 19  | 48    | 198  | GLY  | CA-C-N | 7.66  | 132.35      | 121.02   |
| 19  | 48    | 198  | GLY  | C-N-CA | 7.66  | 132.35      | 121.02   |
| 9   | K8    | 1062 | PRO  | O-C-N  | -7.65 | 112.31      | 122.64   |
| 10  | C16   | 439  | LEU  | CA-C-N | 7.65  | 128.04      | 119.32   |
| 10  | C16   | 439  | LEU  | C-N-CA | 7.65  | 128.04      | 119.32   |
| 9   | K     | 583  | GLU  | O-C-N  | 7.64  | 130.34      | 122.09   |
| 10  | C32   | 664  | ASN  | O-C-N  | 7.64  | 130.22      | 122.12   |
| 10  | C24   | 1060 | ALA  | O-C-N  | -7.64 | 111.60      | 122.29   |
| 18  | B     | 615  | GLU  | CA-C-N | 7.64  | 136.13      | 121.54   |
| 18  | B     | 615  | GLU  | C-N-CA | 7.64  | 136.13      | 121.54   |
| 7   | Q8    | 88   | ASN  | O-C-N  | -7.63 | 112.44      | 122.59   |
| 10  | C8    | 439  | LEU  | CA-C-N | 7.63  | 128.02      | 119.32   |
| 10  | C8    | 439  | LEU  | C-N-CA | 7.63  | 128.02      | 119.32   |
| 18  | B8    | 1803 | THR  | CA-C-N | -7.63 | 106.97      | 121.54   |
| 18  | B8    | 1803 | THR  | C-N-CA | -7.63 | 106.97      | 121.54   |
| 10  | C24   | 253  | ASP  | CA-C-N | 7.63  | 130.50      | 120.28   |
| 10  | C24   | 253  | ASP  | C-N-CA | 7.63  | 130.50      | 120.28   |
| 10  | C16   | 1060 | ALA  | O-C-N  | -7.63 | 111.61      | 122.29   |
| 10  | C8    | 1441 | TYR  | O-C-N  | -7.63 | 112.29      | 122.43   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 464  | ASN  | O-C-N  | 7.62  | 130.20      | 122.12   |
| 9   | K     | 1062 | PRO  | O-C-N  | -7.62 | 112.35      | 122.64   |
| 18  | B8    | 615  | GLU  | CA-C-N | 7.62  | 136.10      | 121.54   |
| 18  | B8    | 615  | GLU  | C-N-CA | 7.62  | 136.10      | 121.54   |
| 10  | C16   | 664  | ASN  | O-C-N  | 7.62  | 130.20      | 122.12   |
| 10  | C8    | 1060 | ALA  | O-C-N  | -7.62 | 111.62      | 122.29   |
| 21  | H16   | 181  | MET  | O-C-N  | -7.62 | 114.16      | 122.85   |
| 7   | Q     | 88   | ASN  | O-C-N  | -7.62 | 112.46      | 122.59   |
| 10  | C24   | 630  | SER  | CA-C-N | 7.61  | 136.07      | 121.54   |
| 10  | C24   | 630  | SER  | C-N-CA | 7.61  | 136.07      | 121.54   |
| 18  | B8    | 1671 | ASP  | O-C-N  | -7.61 | 112.44      | 122.33   |
| 19  | 4     | 198  | GLY  | CA-C-N | 7.61  | 132.28      | 121.02   |
| 19  | 4     | 198  | GLY  | C-N-CA | 7.61  | 132.28      | 121.02   |
| 5   | P     | 5    | SER  | O-C-N  | -7.60 | 112.48      | 122.59   |
| 10  | C     | 1060 | ALA  | O-C-N  | -7.60 | 111.65      | 122.29   |
| 10  | C32   | 1060 | ALA  | O-C-N  | -7.60 | 111.65      | 122.29   |
| 10  | C32   | 630  | SER  | CA-C-N | 7.60  | 136.06      | 121.54   |
| 10  | C32   | 630  | SER  | C-N-CA | 7.60  | 136.06      | 121.54   |
| 11  | A40   | 556  | LYS  | CA-C-N | -7.60 | 109.77      | 121.02   |
| 11  | A40   | 556  | LYS  | C-N-CA | -7.60 | 109.77      | 121.02   |
| 21  | H     | 181  | MET  | O-C-N  | -7.60 | 114.19      | 122.85   |
| 2   | M8    | 386  | ASN  | CA-C-N | 7.59  | 136.30      | 121.41   |
| 2   | M8    | 386  | ASN  | C-N-CA | 7.59  | 136.30      | 121.41   |
| 9   | K8    | 930  | THR  | CA-C-N | 7.59  | 136.04      | 121.54   |
| 9   | K8    | 930  | THR  | C-N-CA | 7.59  | 136.04      | 121.54   |
| 10  | C     | 464  | ASN  | O-C-N  | 7.59  | 130.17      | 122.12   |
| 2   | M     | 386  | ASN  | CA-C-N | 7.59  | 136.28      | 121.41   |
| 2   | M     | 386  | ASN  | C-N-CA | 7.59  | 136.28      | 121.41   |
| 10  | C16   | 630  | SER  | CA-C-N | 7.58  | 136.03      | 121.54   |
| 10  | C16   | 630  | SER  | C-N-CA | 7.58  | 136.03      | 121.54   |
| 10  | C24   | 664  | ASN  | O-C-N  | 7.58  | 130.16      | 122.12   |
| 10  | C24   | 439  | LEU  | CA-C-N | 7.58  | 127.96      | 119.32   |
| 10  | C24   | 439  | LEU  | C-N-CA | 7.58  | 127.96      | 119.32   |
| 18  | B     | 1595 | ASP  | CA-C-N | 7.58  | 136.27      | 121.41   |
| 18  | B     | 1595 | ASP  | C-N-CA | 7.58  | 136.27      | 121.41   |
| 21  | H24   | 181  | MET  | O-C-N  | -7.58 | 114.21      | 122.85   |
| 3   | N     | 166  | ALA  | O-C-N  | -7.58 | 114.71      | 123.27   |
| 10  | C8    | 464  | ASN  | O-C-N  | 7.58  | 130.15      | 122.12   |
| 18  | B8    | 1595 | ASP  | CA-C-N | 7.58  | 136.26      | 121.41   |
| 18  | B8    | 1595 | ASP  | C-N-CA | 7.58  | 136.26      | 121.41   |
| 3   | N8    | 166  | ALA  | O-C-N  | -7.58 | 114.71      | 123.27   |
| 18  | B8    | 1364 | GLU  | O-C-N  | -7.58 | 112.51      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 439  | LEU  | CA-C-N | 7.58  | 127.96      | 119.32   |
| 10  | C32   | 439  | LEU  | C-N-CA | 7.58  | 127.96      | 119.32   |
| 5   | P8    | 5    | SER  | O-C-N  | -7.57 | 112.52      | 122.59   |
| 10  | C     | 630  | SER  | CA-C-N | 7.57  | 135.99      | 121.54   |
| 10  | C     | 630  | SER  | C-N-CA | 7.57  | 135.99      | 121.54   |
| 10  | C8    | 664  | ASN  | O-C-N  | 7.56  | 130.14      | 122.12   |
| 10  | C     | 664  | ASN  | O-C-N  | 7.56  | 130.13      | 122.12   |
| 2   | M16   | 386  | ASN  | CA-C-N | 7.55  | 136.21      | 121.41   |
| 2   | M16   | 386  | ASN  | C-N-CA | 7.55  | 136.21      | 121.41   |
| 9   | K     | 930  | THR  | CA-C-N | 7.55  | 135.96      | 121.54   |
| 9   | K     | 930  | THR  | C-N-CA | 7.55  | 135.96      | 121.54   |
| 17  | F24   | 75   | ALA  | CA-C-N | -7.54 | 109.58      | 120.29   |
| 17  | F24   | 75   | ALA  | C-N-CA | -7.54 | 109.58      | 120.29   |
| 18  | B     | 1364 | GLU  | O-C-N  | -7.54 | 112.56      | 122.59   |
| 5   | P16   | 5    | SER  | O-C-N  | -7.54 | 112.57      | 122.59   |
| 13  | V     | 829  | ARG  | O-C-N  | -7.53 | 114.31      | 122.07   |
| 17  | F8    | 75   | ALA  | CA-C-N | -7.53 | 109.59      | 120.29   |
| 17  | F8    | 75   | ALA  | C-N-CA | -7.53 | 109.59      | 120.29   |
| 3   | N16   | 166  | ALA  | O-C-N  | -7.52 | 114.77      | 123.27   |
| 21  | H8    | 181  | MET  | O-C-N  | -7.52 | 114.28      | 122.85   |
| 10  | C24   | 1496 | PHE  | O-C-N  | -7.51 | 112.26      | 122.48   |
| 10  | C8    | 665  | ALA  | O-C-N  | 7.51  | 130.08      | 122.12   |
| 18  | B8    | 1688 | ALA  | O-C-N  | 7.51  | 130.08      | 122.12   |
| 6   | O     | 163  | LEU  | O-C-N  | -7.51 | 113.06      | 122.82   |
| 10  | C8    | 426  | LEU  | CA-C-N | -7.51 | 110.08      | 122.32   |
| 10  | C8    | 426  | LEU  | C-N-CA | -7.51 | 110.08      | 122.32   |
| 10  | C32   | 665  | ALA  | O-C-N  | 7.51  | 130.08      | 122.12   |
| 17  | F     | 75   | ALA  | CA-C-N | -7.50 | 109.64      | 120.29   |
| 17  | F     | 75   | ALA  | C-N-CA | -7.50 | 109.64      | 120.29   |
| 17  | F16   | 75   | ALA  | CA-C-N | -7.50 | 109.64      | 120.29   |
| 17  | F16   | 75   | ALA  | C-N-CA | -7.50 | 109.64      | 120.29   |
| 2   | M16   | 450  | ASN  | CA-C-N | -7.50 | 110.61      | 122.08   |
| 2   | M16   | 450  | ASN  | C-N-CA | -7.50 | 110.61      | 122.08   |
| 10  | C     | 1496 | PHE  | O-C-N  | -7.50 | 112.28      | 122.48   |
| 10  | C16   | 1496 | PHE  | O-C-N  | -7.49 | 112.29      | 122.48   |
| 10  | C24   | 464  | ASN  | O-C-N  | 7.49  | 130.06      | 122.12   |
| 6   | O8    | 163  | LEU  | O-C-N  | -7.49 | 113.08      | 122.82   |
| 6   | O16   | 163  | LEU  | O-C-N  | -7.49 | 113.09      | 122.82   |
| 18  | B8    | 856  | LEU  | O-C-N  | -7.49 | 112.71      | 121.32   |
| 18  | B8    | 1793 | ILE  | CA-C-N | -7.48 | 107.25      | 121.54   |
| 18  | B8    | 1793 | ILE  | C-N-CA | -7.48 | 107.25      | 121.54   |
| 14  | W     | 705  | HIS  | O-C-N  | -7.48 | 112.09      | 122.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 849  | SER  | CA-C-N | -7.47 | 101.00      | 122.15   |
| 10  | C24   | 849  | SER  | C-N-CA | -7.47 | 101.00      | 122.15   |
| 18  | B8    | 939  | SER  | O-C-N  | -7.47 | 113.69      | 122.87   |
| 18  | B     | 1688 | ALA  | O-C-N  | 7.46  | 130.03      | 122.12   |
| 10  | C24   | 426  | LEU  | CA-C-N | -7.46 | 110.16      | 122.32   |
| 10  | C24   | 426  | LEU  | C-N-CA | -7.46 | 110.16      | 122.32   |
| 2   | M     | 450  | ASN  | CA-C-N | -7.46 | 110.66      | 122.08   |
| 2   | M     | 450  | ASN  | C-N-CA | -7.46 | 110.66      | 122.08   |
| 18  | B     | 939  | SER  | O-C-N  | -7.45 | 113.70      | 122.87   |
| 10  | C16   | 849  | SER  | CA-C-N | -7.45 | 101.06      | 122.15   |
| 10  | C16   | 849  | SER  | C-N-CA | -7.45 | 101.06      | 122.15   |
| 10  | C8    | 1496 | PHE  | O-C-N  | -7.45 | 112.35      | 122.48   |
| 14  | W     | 586  | ILE  | O-C-N  | -7.45 | 115.03      | 122.93   |
| 10  | C32   | 849  | SER  | CA-C-N | -7.45 | 101.07      | 122.15   |
| 10  | C32   | 849  | SER  | C-N-CA | -7.45 | 101.07      | 122.15   |
| 10  | C     | 849  | SER  | CA-C-N | -7.45 | 101.07      | 122.15   |
| 10  | C     | 849  | SER  | C-N-CA | -7.45 | 101.07      | 122.15   |
| 9   | K8    | 1284 | MET  | CA-C-N | -7.45 | 108.30      | 121.70   |
| 9   | K8    | 1284 | MET  | C-N-CA | -7.45 | 108.30      | 121.70   |
| 10  | C8    | 849  | SER  | CA-C-N | -7.45 | 101.08      | 122.15   |
| 10  | C8    | 849  | SER  | C-N-CA | -7.45 | 101.08      | 122.15   |
| 2   | M8    | 450  | ASN  | CA-C-N | -7.44 | 110.69      | 122.08   |
| 2   | M8    | 450  | ASN  | C-N-CA | -7.44 | 110.69      | 122.08   |
| 10  | C16   | 426  | LEU  | CA-C-N | -7.44 | 110.19      | 122.32   |
| 10  | C16   | 426  | LEU  | C-N-CA | -7.44 | 110.19      | 122.32   |
| 18  | B     | 1793 | ILE  | CA-C-N | -7.44 | 107.33      | 121.54   |
| 18  | B     | 1793 | ILE  | C-N-CA | -7.44 | 107.33      | 121.54   |
| 1   | R8    | 1194 | ARG  | CA-C-N | -7.43 | 110.84      | 120.65   |
| 1   | R8    | 1194 | ARG  | C-N-CA | -7.43 | 110.84      | 120.65   |
| 1   | R     | 1194 | ARG  | CA-C-N | -7.43 | 110.84      | 120.65   |
| 1   | R     | 1194 | ARG  | C-N-CA | -7.43 | 110.84      | 120.65   |
| 1   | R8    | 1325 | GLN  | CA-C-N | 7.43  | 128.23      | 119.98   |
| 1   | R8    | 1325 | GLN  | C-N-CA | 7.43  | 128.23      | 119.98   |
| 9   | K     | 984  | GLY  | CA-C-N | 7.43  | 130.98      | 120.28   |
| 9   | K     | 984  | GLY  | C-N-CA | 7.43  | 130.98      | 120.28   |
| 18  | B8    | 599  | ILE  | O-C-N  | -7.43 | 113.59      | 122.06   |
| 9   | K     | 1284 | MET  | CA-C-N | -7.43 | 108.33      | 121.70   |
| 9   | K     | 1284 | MET  | C-N-CA | -7.43 | 108.33      | 121.70   |
| 10  | C32   | 1496 | PHE  | O-C-N  | -7.43 | 112.38      | 122.48   |
| 9   | K8    | 748  | THR  | CA-C-N | 7.42  | 132.20      | 120.47   |
| 9   | K8    | 748  | THR  | C-N-CA | 7.42  | 132.20      | 120.47   |
| 1   | R     | 1325 | GLN  | CA-C-N | 7.42  | 128.22      | 119.98   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | R     | 1325 | GLN  | C-N-CA | 7.42  | 128.22      | 119.98   |
| 10  | C16   | 1707 | SER  | O-C-N  | -7.42 | 114.10      | 122.86   |
| 18  | B     | 856  | LEU  | O-C-N  | -7.42 | 112.79      | 121.32   |
| 1   | R16   | 1204 | ASN  | O-C-N  | -7.42 | 112.73      | 122.59   |
| 10  | C16   | 665  | ALA  | O-C-N  | 7.42  | 129.98      | 122.12   |
| 1   | R     | 1204 | ASN  | O-C-N  | -7.42 | 112.73      | 122.59   |
| 18  | B8    | 1392 | SER  | CA-C-N | -7.41 | 112.67      | 123.05   |
| 18  | B8    | 1392 | SER  | C-N-CA | -7.41 | 112.67      | 123.05   |
| 22  | I16   | 154  | GLU  | O-C-N  | 7.41  | 129.97      | 122.12   |
| 10  | C     | 665  | ALA  | O-C-N  | 7.41  | 129.97      | 122.12   |
| 22  | I8    | 154  | GLU  | O-C-N  | 7.41  | 129.97      | 122.12   |
| 10  | C16   | 1619 | PRO  | CA-C-N | -7.41 | 108.64      | 121.97   |
| 10  | C16   | 1619 | PRO  | C-N-CA | -7.41 | 108.64      | 121.97   |
| 10  | C16   | 1707 | SER  | CA-C-N | 7.41  | 130.53      | 120.38   |
| 10  | C16   | 1707 | SER  | C-N-CA | 7.41  | 130.53      | 120.38   |
| 10  | C24   | 1707 | SER  | CA-C-N | 7.41  | 130.53      | 120.38   |
| 10  | C24   | 1707 | SER  | C-N-CA | 7.41  | 130.53      | 120.38   |
| 10  | C8    | 1619 | PRO  | CA-C-N | -7.41 | 108.64      | 121.97   |
| 10  | C8    | 1619 | PRO  | C-N-CA | -7.41 | 108.64      | 121.97   |
| 18  | B     | 599  | ILE  | O-C-N  | -7.41 | 113.62      | 122.06   |
| 10  | C     | 426  | LEU  | CA-C-N | -7.40 | 110.25      | 122.32   |
| 10  | C     | 426  | LEU  | C-N-CA | -7.40 | 110.25      | 122.32   |
| 9   | K8    | 984  | GLY  | CA-C-N | 7.40  | 130.94      | 120.28   |
| 9   | K8    | 984  | GLY  | C-N-CA | 7.40  | 130.94      | 120.28   |
| 23  | J24   | 724  | GLY  | CA-C-N | 7.40  | 132.34      | 121.31   |
| 23  | J24   | 724  | GLY  | C-N-CA | 7.40  | 132.34      | 121.31   |
| 9   | K     | 748  | THR  | CA-C-N | 7.40  | 132.16      | 120.47   |
| 9   | K     | 748  | THR  | C-N-CA | 7.40  | 132.16      | 120.47   |
| 1   | R16   | 1325 | GLN  | CA-C-N | 7.40  | 128.19      | 119.98   |
| 1   | R16   | 1325 | GLN  | C-N-CA | 7.40  | 128.19      | 119.98   |
| 19  | 48    | 102  | LEU  | O-C-N  | -7.39 | 111.94      | 122.29   |
| 10  | C32   | 426  | LEU  | CA-C-N | -7.39 | 110.27      | 122.32   |
| 10  | C32   | 426  | LEU  | C-N-CA | -7.39 | 110.27      | 122.32   |
| 1   | R8    | 1204 | ASN  | O-C-N  | -7.39 | 112.77      | 122.59   |
| 19  | 4     | 102  | LEU  | O-C-N  | -7.39 | 111.95      | 122.29   |
| 23  | J8    | 724  | GLY  | CA-C-N | 7.39  | 132.32      | 121.31   |
| 23  | J8    | 724  | GLY  | C-N-CA | 7.39  | 132.32      | 121.31   |
| 22  | I24   | 154  | GLU  | O-C-N  | 7.39  | 129.95      | 122.12   |
| 10  | C8    | 1509 | SER  | CA-C-N | 7.38  | 135.65      | 121.54   |
| 10  | C8    | 1509 | SER  | C-N-CA | 7.38  | 135.65      | 121.54   |
| 23  | J16   | 724  | GLY  | CA-C-N | 7.38  | 132.31      | 121.31   |
| 23  | J16   | 724  | GLY  | C-N-CA | 7.38  | 132.31      | 121.31   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22  | I     | 154  | GLU  | O-C-N  | 7.38  | 129.95      | 122.12   |
| 10  | C     | 1619 | PRO  | CA-C-N | -7.37 | 108.70      | 121.97   |
| 10  | C     | 1619 | PRO  | C-N-CA | -7.37 | 108.70      | 121.97   |
| 1   | R16   | 1376 | LYS  | CA-C-N | 7.37  | 132.39      | 120.60   |
| 1   | R16   | 1376 | LYS  | C-N-CA | 7.37  | 132.39      | 120.60   |
| 10  | C32   | 1619 | PRO  | CA-C-N | -7.37 | 108.71      | 121.97   |
| 10  | C32   | 1619 | PRO  | C-N-CA | -7.37 | 108.71      | 121.97   |
| 10  | C     | 1509 | SER  | CA-C-N | 7.37  | 135.61      | 121.54   |
| 10  | C     | 1509 | SER  | C-N-CA | 7.37  | 135.61      | 121.54   |
| 1   | R16   | 1194 | ARG  | CA-C-N | -7.36 | 110.93      | 120.65   |
| 1   | R16   | 1194 | ARG  | C-N-CA | -7.36 | 110.93      | 120.65   |
| 10  | C16   | 661  | ASN  | O-C-N  | 7.36  | 129.93      | 122.12   |
| 10  | C32   | 1509 | SER  | CA-C-N | 7.36  | 135.61      | 121.54   |
| 10  | C32   | 1509 | SER  | C-N-CA | 7.36  | 135.61      | 121.54   |
| 18  | B8    | 1481 | MET  | O-C-N  | -7.36 | 114.44      | 122.09   |
| 10  | C24   | 1509 | SER  | CA-C-N | 7.36  | 135.60      | 121.54   |
| 10  | C24   | 1509 | SER  | C-N-CA | 7.36  | 135.60      | 121.54   |
| 18  | B     | 1392 | SER  | CA-C-N | -7.36 | 112.75      | 123.05   |
| 18  | B     | 1392 | SER  | C-N-CA | -7.36 | 112.75      | 123.05   |
| 9   | K     | 1020 | HIS  | O-C-N  | 7.35  | 130.43      | 122.64   |
| 10  | C16   | 1509 | SER  | CA-C-N | 7.35  | 135.58      | 121.54   |
| 10  | C16   | 1509 | SER  | C-N-CA | 7.35  | 135.58      | 121.54   |
| 1   | R8    | 1376 | LYS  | CA-C-N | 7.35  | 132.36      | 120.60   |
| 1   | R8    | 1376 | LYS  | C-N-CA | 7.35  | 132.36      | 120.60   |
| 23  | J16   | 734  | PRO  | CA-C-N | -7.35 | 109.65      | 120.38   |
| 23  | J16   | 734  | PRO  | C-N-CA | -7.35 | 109.65      | 120.38   |
| 23  | J24   | 734  | PRO  | CA-C-N | -7.35 | 109.66      | 120.38   |
| 23  | J24   | 734  | PRO  | C-N-CA | -7.35 | 109.66      | 120.38   |
| 23  | J32   | 734  | PRO  | CA-C-N | -7.34 | 109.66      | 120.38   |
| 23  | J32   | 734  | PRO  | C-N-CA | -7.34 | 109.66      | 120.38   |
| 10  | C32   | 1707 | SER  | O-C-N  | -7.34 | 114.19      | 122.86   |
| 10  | C24   | 1619 | PRO  | CA-C-N | -7.34 | 108.76      | 121.97   |
| 10  | C24   | 1619 | PRO  | C-N-CA | -7.34 | 108.76      | 121.97   |
| 18  | B8    | 552  | SER  | O-C-N  | -7.34 | 112.83      | 122.59   |
| 1   | R     | 1376 | LYS  | CA-C-N | 7.34  | 132.34      | 120.60   |
| 1   | R     | 1376 | LYS  | C-N-CA | 7.34  | 132.34      | 120.60   |
| 15  | J     | 659  | GLU  | O-C-N  | 7.34  | 130.52      | 122.15   |
| 23  | J8    | 734  | PRO  | CA-C-N | -7.34 | 109.67      | 120.38   |
| 23  | J8    | 734  | PRO  | C-N-CA | -7.34 | 109.67      | 120.38   |
| 10  | C24   | 1707 | SER  | O-C-N  | -7.34 | 114.20      | 122.86   |
| 23  | J32   | 724  | GLY  | CA-C-N | 7.34  | 132.24      | 121.31   |
| 23  | J32   | 724  | GLY  | C-N-CA | 7.34  | 132.24      | 121.31   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C     | 1707 | SER  | CA-C-N | 7.33  | 130.43      | 120.38   |
| 10  | C     | 1707 | SER  | C-N-CA | 7.33  | 130.43      | 120.38   |
| 5   | P8    | 3    | GLY  | CA-C-N | 7.33  | 135.54      | 121.54   |
| 5   | P8    | 3    | GLY  | C-N-CA | 7.33  | 135.54      | 121.54   |
| 9   | K8    | 1020 | HIS  | O-C-N  | 7.33  | 130.41      | 122.64   |
| 5   | P     | 3    | GLY  | CA-C-N | 7.33  | 135.54      | 121.54   |
| 5   | P     | 3    | GLY  | C-N-CA | 7.33  | 135.54      | 121.54   |
| 18  | B8    | 505  | ALA  | O-C-N  | -7.33 | 114.41      | 122.03   |
| 10  | C32   | 1707 | SER  | CA-C-N | 7.33  | 130.42      | 120.38   |
| 10  | C32   | 1707 | SER  | C-N-CA | 7.33  | 130.42      | 120.38   |
| 3   | N8    | 172  | LEU  | CA-C-N | -7.32 | 111.87      | 122.19   |
| 3   | N8    | 172  | LEU  | C-N-CA | -7.32 | 111.87      | 122.19   |
| 14  | W     | 586  | ILE  | CA-C-N | 7.32  | 131.20      | 120.95   |
| 14  | W     | 586  | ILE  | C-N-CA | 7.32  | 131.20      | 120.95   |
| 10  | C8    | 1707 | SER  | CA-C-N | 7.31  | 130.39      | 120.38   |
| 10  | C8    | 1707 | SER  | C-N-CA | 7.31  | 130.39      | 120.38   |
| 18  | B     | 552  | SER  | O-C-N  | -7.31 | 112.87      | 122.59   |
| 10  | C     | 1507 | LEU  | O-C-N  | -7.30 | 112.33      | 122.41   |
| 18  | B     | 1481 | MET  | O-C-N  | -7.30 | 114.50      | 122.09   |
| 18  | B     | 505  | ALA  | O-C-N  | -7.30 | 114.44      | 122.03   |
| 5   | P16   | 3    | GLY  | CA-C-N | 7.29  | 135.47      | 121.54   |
| 5   | P16   | 3    | GLY  | C-N-CA | 7.29  | 135.47      | 121.54   |
| 5   | P     | 658  | PRO  | O-C-N  | -7.29 | 113.12      | 122.23   |
| 5   | P8    | 658  | PRO  | O-C-N  | -7.28 | 113.13      | 122.23   |
| 10  | C     | 1707 | SER  | O-C-N  | -7.28 | 114.27      | 122.86   |
| 18  | B     | 883  | TYR  | O-C-N  | -7.28 | 113.44      | 122.68   |
| 10  | C24   | 661  | ASN  | O-C-N  | 7.27  | 129.83      | 122.12   |
| 10  | C8    | 661  | ASN  | O-C-N  | 7.27  | 129.82      | 122.12   |
| 23  | J8    | 685  | GLY  | CA-C-N | -7.27 | 111.03      | 121.42   |
| 23  | J8    | 685  | GLY  | C-N-CA | -7.27 | 111.03      | 121.42   |
| 13  | V     | 812  | GLU  | O-C-N  | 7.27  | 129.82      | 122.12   |
| 10  | C32   | 1032 | THR  | CA-C-N | 7.27  | 133.73      | 120.79   |
| 10  | C32   | 1032 | THR  | C-N-CA | 7.27  | 133.73      | 120.79   |
| 10  | C8    | 1507 | LEU  | O-C-N  | -7.27 | 112.38      | 122.41   |
| 3   | N     | 172  | LEU  | CA-C-N | -7.26 | 111.95      | 122.19   |
| 3   | N     | 172  | LEU  | C-N-CA | -7.26 | 111.95      | 122.19   |
| 10  | C     | 1032 | THR  | CA-C-N | 7.26  | 133.72      | 120.79   |
| 10  | C     | 1032 | THR  | C-N-CA | 7.26  | 133.72      | 120.79   |
| 5   | P16   | 658  | PRO  | O-C-N  | -7.26 | 113.15      | 122.23   |
| 10  | C32   | 1507 | LEU  | O-C-N  | -7.26 | 112.39      | 122.41   |
| 10  | C32   | 427  | ASP  | CA-C-N | 7.26  | 135.63      | 121.41   |
| 10  | C32   | 427  | ASP  | C-N-CA | 7.26  | 135.63      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | N16   | 172  | LEU  | CA-C-N | -7.25 | 111.96      | 122.19   |
| 3   | N16   | 172  | LEU  | C-N-CA | -7.25 | 111.96      | 122.19   |
| 9   | K8    | 1054 | THR  | CA-C-N | 7.25  | 136.82      | 122.31   |
| 9   | K8    | 1054 | THR  | C-N-CA | 7.25  | 136.82      | 122.31   |
| 20  | E     | 433  | LYS  | CA-C-N | -7.25 | 107.69      | 121.54   |
| 20  | E     | 433  | LYS  | C-N-CA | -7.25 | 107.69      | 121.54   |
| 10  | C16   | 427  | ASP  | CA-C-N | 7.25  | 135.62      | 121.41   |
| 10  | C16   | 427  | ASP  | C-N-CA | 7.25  | 135.62      | 121.41   |
| 18  | B8    | 1418 | ALA  | O-C-N  | -7.25 | 113.28      | 122.34   |
| 19  | 48    | 372  | LYS  | O-C-N  | 7.25  | 131.57      | 123.16   |
| 10  | C32   | 661  | ASN  | O-C-N  | 7.25  | 129.80      | 122.12   |
| 10  | C8    | 1707 | SER  | O-C-N  | -7.25 | 114.31      | 122.86   |
| 10  | C24   | 1032 | THR  | CA-C-N | 7.24  | 133.68      | 120.79   |
| 10  | C24   | 1032 | THR  | C-N-CA | 7.24  | 133.68      | 120.79   |
| 10  | C32   | 1659 | ASP  | CA-C-N | -7.24 | 110.51      | 122.32   |
| 10  | C32   | 1659 | ASP  | C-N-CA | -7.24 | 110.51      | 122.32   |
| 9   | K8    | 639  | THR  | O-C-N  | -7.24 | 113.00      | 122.77   |
| 10  | C16   | 1507 | LEU  | O-C-N  | -7.24 | 112.42      | 122.41   |
| 10  | C     | 661  | ASN  | O-C-N  | 7.24  | 129.79      | 122.12   |
| 9   | K     | 1054 | THR  | CA-C-N | 7.24  | 136.78      | 122.31   |
| 9   | K     | 1054 | THR  | C-N-CA | 7.24  | 136.78      | 122.31   |
| 10  | C16   | 1032 | THR  | CA-C-N | 7.24  | 133.67      | 120.79   |
| 10  | C16   | 1032 | THR  | C-N-CA | 7.24  | 133.67      | 120.79   |
| 10  | C     | 666  | LEU  | O-C-N  | 7.24  | 131.64      | 122.23   |
| 5   | P     | 16   | PHE  | O-C-N  | -7.23 | 112.14      | 122.41   |
| 10  | C8    | 1032 | THR  | CA-C-N | 7.23  | 133.66      | 120.79   |
| 10  | C8    | 1032 | THR  | C-N-CA | 7.23  | 133.66      | 120.79   |
| 18  | B     | 1418 | ALA  | O-C-N  | -7.23 | 113.30      | 122.34   |
| 20  | E8    | 433  | LYS  | CA-C-N | -7.23 | 107.73      | 121.54   |
| 20  | E8    | 433  | LYS  | C-N-CA | -7.23 | 107.73      | 121.54   |
| 14  | W     | 763  | TYR  | CA-C-N | -7.23 | 111.04      | 120.44   |
| 14  | W     | 763  | TYR  | C-N-CA | -7.23 | 111.04      | 120.44   |
| 22  | I     | 368  | VAL  | O-C-N  | -7.23 | 114.20      | 121.94   |
| 5   | P16   | 16   | PHE  | O-C-N  | -7.23 | 112.15      | 122.41   |
| 10  | C     | 427  | ASP  | CA-C-N | 7.23  | 135.58      | 121.41   |
| 10  | C     | 427  | ASP  | C-N-CA | 7.23  | 135.58      | 121.41   |
| 18  | B8    | 883  | TYR  | O-C-N  | -7.23 | 113.50      | 122.68   |
| 10  | C8    | 427  | ASP  | CA-C-N | 7.22  | 135.57      | 121.41   |
| 10  | C8    | 427  | ASP  | C-N-CA | 7.22  | 135.57      | 121.41   |
| 19  | 4     | 372  | LYS  | O-C-N  | 7.22  | 131.54      | 123.16   |
| 10  | C24   | 427  | ASP  | CA-C-N | 7.22  | 135.56      | 121.41   |
| 10  | C24   | 427  | ASP  | C-N-CA | 7.22  | 135.56      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B8    | 413  | ASP  | CA-C-N | 7.22  | 135.56      | 121.41   |
| 18  | B8    | 413  | ASP  | C-N-CA | 7.22  | 135.56      | 121.41   |
| 14  | W     | 599  | ALA  | O-C-N  | -7.22 | 114.87      | 121.30   |
| 18  | B     | 413  | ASP  | CA-C-N | 7.22  | 135.56      | 121.41   |
| 18  | B     | 413  | ASP  | C-N-CA | 7.22  | 135.56      | 121.41   |
| 22  | I8    | 368  | VAL  | O-C-N  | -7.21 | 114.22      | 121.94   |
| 10  | C24   | 1659 | ASP  | CA-C-N | -7.21 | 110.56      | 122.32   |
| 10  | C24   | 1659 | ASP  | C-N-CA | -7.21 | 110.56      | 122.32   |
| 22  | I24   | 368  | VAL  | O-C-N  | -7.21 | 114.23      | 121.94   |
| 10  | C     | 334  | MET  | CA-C-N | 7.21  | 135.30      | 121.54   |
| 10  | C     | 334  | MET  | C-N-CA | 7.21  | 135.30      | 121.54   |
| 19  | 48    | 69   | GLU  | CA-C-N | -7.21 | 107.53      | 121.58   |
| 19  | 48    | 69   | GLU  | C-N-CA | -7.21 | 107.53      | 121.58   |
| 22  | I16   | 368  | VAL  | O-C-N  | -7.20 | 114.23      | 121.94   |
| 19  | 4     | 69   | GLU  | CA-C-N | -7.20 | 107.54      | 121.58   |
| 19  | 4     | 69   | GLU  | C-N-CA | -7.20 | 107.54      | 121.58   |
| 23  | J16   | 685  | GLY  | CA-C-N | -7.20 | 111.12      | 121.42   |
| 23  | J16   | 685  | GLY  | C-N-CA | -7.20 | 111.12      | 121.42   |
| 5   | P8    | 16   | PHE  | O-C-N  | -7.20 | 112.19      | 122.41   |
| 10  | C32   | 334  | MET  | CA-C-N | 7.20  | 135.29      | 121.54   |
| 10  | C32   | 334  | MET  | C-N-CA | 7.20  | 135.29      | 121.54   |
| 12  | A     | 552  | GLY  | CA-C-N | 7.20  | 135.28      | 121.54   |
| 12  | A     | 552  | GLY  | C-N-CA | 7.20  | 135.28      | 121.54   |
| 10  | C24   | 1507 | LEU  | O-C-N  | -7.19 | 112.48      | 122.41   |
| 9   | K     | 639  | THR  | O-C-N  | -7.19 | 113.06      | 122.77   |
| 10  | C     | 1659 | ASP  | CA-C-N | -7.19 | 110.60      | 122.32   |
| 10  | C     | 1659 | ASP  | C-N-CA | -7.19 | 110.60      | 122.32   |
| 23  | J24   | 685  | GLY  | CA-C-N | -7.19 | 111.13      | 121.42   |
| 23  | J24   | 685  | GLY  | C-N-CA | -7.19 | 111.13      | 121.42   |
| 18  | B8    | 1114 | CYS  | O-C-N  | -7.19 | 115.06      | 123.11   |
| 9   | K     | 1278 | GLU  | CA-C-N | 7.19  | 131.23      | 120.31   |
| 9   | K     | 1278 | GLU  | C-N-CA | 7.19  | 131.23      | 120.31   |
| 10  | C32   | 1665 | THR  | O-C-N  | -7.18 | 113.36      | 122.34   |
| 23  | J32   | 685  | GLY  | CA-C-N | -7.18 | 111.15      | 121.42   |
| 23  | J32   | 685  | GLY  | C-N-CA | -7.18 | 111.15      | 121.42   |
| 11  | A24   | 552  | GLY  | CA-C-N | 7.18  | 135.25      | 121.54   |
| 11  | A24   | 552  | GLY  | C-N-CA | 7.18  | 135.25      | 121.54   |
| 11  | A40   | 552  | GLY  | CA-C-N | 7.18  | 135.25      | 121.54   |
| 11  | A40   | 552  | GLY  | C-N-CA | 7.18  | 135.25      | 121.54   |
| 10  | C16   | 1659 | ASP  | CA-C-N | -7.17 | 110.62      | 122.32   |
| 10  | C16   | 1659 | ASP  | C-N-CA | -7.17 | 110.62      | 122.32   |
| 10  | C24   | 334  | MET  | CA-C-N | 7.17  | 135.24      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 334  | MET  | C-N-CA | 7.17  | 135.24      | 121.54   |
| 18  | B     | 1602 | SER  | CA-C-N | 7.17  | 132.60      | 121.19   |
| 18  | B     | 1602 | SER  | C-N-CA | 7.17  | 132.60      | 121.19   |
| 10  | C8    | 334  | MET  | CA-C-N | 7.17  | 135.23      | 121.54   |
| 10  | C8    | 334  | MET  | C-N-CA | 7.17  | 135.23      | 121.54   |
| 12  | A48   | 552  | GLY  | CA-C-N | 7.17  | 135.23      | 121.54   |
| 12  | A48   | 552  | GLY  | C-N-CA | 7.17  | 135.23      | 121.54   |
| 13  | V     | 875  | HIS  | O-C-N  | -7.17 | 113.08      | 121.32   |
| 18  | B     | 507  | ASP  | CA-C-N | -7.17 | 110.64      | 122.32   |
| 18  | B     | 507  | ASP  | C-N-CA | -7.17 | 110.64      | 122.32   |
| 10  | C32   | 666  | LEU  | O-C-N  | 7.17  | 131.55      | 122.23   |
| 23  | J24   | 723  | GLN  | CA-C-N | 7.17  | 128.03      | 120.43   |
| 23  | J24   | 723  | GLN  | C-N-CA | 7.17  | 128.03      | 120.43   |
| 10  | C24   | 1665 | THR  | O-C-N  | -7.16 | 113.39      | 122.34   |
| 11  | A32   | 552  | GLY  | CA-C-N | 7.16  | 135.22      | 121.54   |
| 11  | A32   | 552  | GLY  | C-N-CA | 7.16  | 135.22      | 121.54   |
| 10  | C16   | 334  | MET  | CA-C-N | 7.16  | 135.22      | 121.54   |
| 10  | C16   | 334  | MET  | C-N-CA | 7.16  | 135.22      | 121.54   |
| 9   | K8    | 1278 | GLU  | CA-C-N | 7.16  | 131.19      | 120.31   |
| 9   | K8    | 1278 | GLU  | C-N-CA | 7.16  | 131.19      | 120.31   |
| 10  | C8    | 666  | LEU  | O-C-N  | 7.16  | 131.53      | 122.23   |
| 11  | A16   | 5    | GLN  | O-C-N  | 7.16  | 131.07      | 122.27   |
| 11  | A32   | 5    | GLN  | O-C-N  | 7.16  | 131.07      | 122.27   |
| 9   | K     | 967  | ASP  | O-C-N  | -7.16 | 113.59      | 122.68   |
| 11  | A24   | 5    | GLN  | O-C-N  | 7.16  | 131.07      | 122.27   |
| 11  | A40   | 5    | GLN  | O-C-N  | 7.15  | 131.07      | 122.27   |
| 18  | B     | 1355 | ASN  | CA-C-N | 7.15  | 130.58      | 120.28   |
| 18  | B     | 1355 | ASN  | C-N-CA | 7.15  | 130.58      | 120.28   |
| 9   | K8    | 967  | ASP  | O-C-N  | -7.15 | 113.60      | 122.68   |
| 10  | C16   | 1665 | THR  | O-C-N  | -7.15 | 113.40      | 122.34   |
| 18  | B8    | 507  | ASP  | CA-C-N | -7.15 | 110.67      | 122.32   |
| 18  | B8    | 507  | ASP  | C-N-CA | -7.15 | 110.67      | 122.32   |
| 11  | A16   | 552  | GLY  | CA-C-N | 7.15  | 135.19      | 121.54   |
| 11  | A16   | 552  | GLY  | C-N-CA | 7.15  | 135.19      | 121.54   |
| 18  | B     | 1114 | CYS  | O-C-N  | -7.14 | 115.11      | 123.11   |
| 1   | R16   | 1198 | GLU  | CA-C-N | -7.14 | 111.16      | 120.44   |
| 1   | R16   | 1198 | GLU  | C-N-CA | -7.14 | 111.16      | 120.44   |
| 18  | B     | 1883 | TYR  | O-C-N  | -7.14 | 113.06      | 122.20   |
| 2   | M16   | 157  | GLY  | CA-C-N | 7.13  | 130.94      | 120.95   |
| 2   | M16   | 157  | GLY  | C-N-CA | 7.13  | 130.94      | 120.95   |
| 18  | B8    | 1883 | TYR  | O-C-N  | -7.13 | 113.07      | 122.20   |
| 23  | J16   | 723  | GLN  | CA-C-N | 7.13  | 127.99      | 120.43   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 23  | J16   | 723  | GLN  | C-N-CA | 7.13  | 127.99      | 120.43   |
| 10  | C16   | 666  | LEU  | O-C-N  | 7.13  | 131.50      | 122.23   |
| 18  | B8    | 1602 | SER  | CA-C-N | 7.13  | 132.53      | 121.19   |
| 18  | B8    | 1602 | SER  | C-N-CA | 7.13  | 132.53      | 121.19   |
| 9   | K     | 1251 | HIS  | O-C-N  | -7.12 | 114.61      | 123.01   |
| 23  | J8    | 723  | GLN  | CA-C-N | 7.12  | 127.97      | 120.43   |
| 23  | J8    | 723  | GLN  | C-N-CA | 7.12  | 127.97      | 120.43   |
| 9   | K     | 731  | CYS  | O-C-N  | -7.12 | 115.14      | 123.11   |
| 10  | C8    | 454  | SER  | CA-C-N | 7.12  | 132.99      | 122.10   |
| 10  | C8    | 454  | SER  | C-N-CA | 7.12  | 132.99      | 122.10   |
| 2   | M     | 157  | GLY  | CA-C-N | 7.11  | 130.91      | 120.95   |
| 2   | M     | 157  | GLY  | C-N-CA | 7.11  | 130.91      | 120.95   |
| 11  | A16   | 243  | ARG  | O-C-N  | -7.11 | 113.14      | 122.59   |
| 2   | M16   | 203  | PRO  | CA-C-N | 7.11  | 130.55      | 120.53   |
| 2   | M16   | 203  | PRO  | C-N-CA | 7.11  | 130.55      | 120.53   |
| 10  | C     | 454  | SER  | CA-C-N | 7.11  | 132.97      | 122.10   |
| 10  | C     | 454  | SER  | C-N-CA | 7.11  | 132.97      | 122.10   |
| 11  | A32   | 243  | ARG  | O-C-N  | -7.10 | 113.14      | 122.59   |
| 10  | C     | 1665 | THR  | O-C-N  | -7.10 | 113.46      | 122.34   |
| 18  | B8    | 1355 | ASN  | CA-C-N | 7.10  | 130.50      | 120.28   |
| 18  | B8    | 1355 | ASN  | C-N-CA | 7.10  | 130.50      | 120.28   |
| 23  | J32   | 723  | GLN  | CA-C-N | 7.10  | 127.95      | 120.43   |
| 23  | J32   | 723  | GLN  | C-N-CA | 7.10  | 127.95      | 120.43   |
| 9   | K8    | 1251 | HIS  | O-C-N  | -7.09 | 114.64      | 123.01   |
| 11  | A24   | 243  | ARG  | O-C-N  | -7.09 | 113.16      | 122.59   |
| 14  | W     | 585  | ILE  | CA-C-N | 7.09  | 133.05      | 122.91   |
| 14  | W     | 585  | ILE  | C-N-CA | 7.09  | 133.05      | 122.91   |
| 10  | C24   | 620  | PRO  | O-C-N  | -7.09 | 113.07      | 122.64   |
| 10  | C     | 620  | PRO  | O-C-N  | -7.09 | 113.07      | 122.64   |
| 10  | C16   | 454  | SER  | CA-C-N | 7.09  | 132.94      | 122.10   |
| 10  | C16   | 454  | SER  | C-N-CA | 7.09  | 132.94      | 122.10   |
| 10  | C8    | 774  | GLY  | O-C-N  | -7.08 | 115.30      | 122.17   |
| 20  | E     | 205  | GLY  | CA-C-N | 7.08  | 135.29      | 121.41   |
| 20  | E     | 205  | GLY  | C-N-CA | 7.08  | 135.29      | 121.41   |
| 9   | K8    | 731  | CYS  | O-C-N  | -7.08 | 115.18      | 123.11   |
| 12  | A48   | 243  | ARG  | O-C-N  | -7.08 | 113.17      | 122.59   |
| 18  | B     | 1673 | ARG  | CA-C-N | -7.08 | 111.24      | 120.44   |
| 18  | B     | 1673 | ARG  | C-N-CA | -7.08 | 111.24      | 120.44   |
| 10  | C24   | 666  | LEU  | O-C-N  | 7.08  | 131.43      | 122.23   |
| 1   | R8    | 1198 | GLU  | CA-C-N | -7.08 | 111.24      | 120.44   |
| 1   | R8    | 1198 | GLU  | C-N-CA | -7.08 | 111.24      | 120.44   |
| 10  | C8    | 620  | PRO  | O-C-N  | -7.08 | 113.09      | 122.64   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 620  | PRO  | O-C-N  | -7.08 | 113.09      | 122.64   |
| 20  | E8    | 205  | GLY  | CA-C-N | 7.08  | 135.28      | 121.41   |
| 20  | E8    | 205  | GLY  | C-N-CA | 7.08  | 135.28      | 121.41   |
| 2   | M8    | 157  | GLY  | CA-C-N | 7.07  | 130.85      | 120.95   |
| 2   | M8    | 157  | GLY  | C-N-CA | 7.07  | 130.85      | 120.95   |
| 5   | P     | 648  | LEU  | O-C-N  | 7.07  | 130.21      | 122.15   |
| 10  | C16   | 1084 | LYS  | O-C-N  | -7.07 | 113.18      | 122.59   |
| 10  | C32   | 620  | PRO  | O-C-N  | -7.07 | 113.09      | 122.64   |
| 11  | A40   | 243  | ARG  | O-C-N  | -7.07 | 113.19      | 122.59   |
| 12  | A     | 243  | ARG  | O-C-N  | -7.07 | 113.19      | 122.59   |
| 10  | C32   | 640  | GLN  | O-C-N  | 7.07  | 129.35      | 122.07   |
| 2   | M8    | 203  | PRO  | CA-C-N | 7.07  | 130.49      | 120.53   |
| 2   | M8    | 203  | PRO  | C-N-CA | 7.07  | 130.49      | 120.53   |
| 10  | C8    | 1084 | LYS  | O-C-N  | -7.06 | 113.19      | 122.59   |
| 2   | M     | 203  | PRO  | CA-C-N | 7.06  | 130.49      | 120.53   |
| 2   | M     | 203  | PRO  | C-N-CA | 7.06  | 130.49      | 120.53   |
| 18  | B     | 975  | ASP  | O-C-N  | -7.06 | 112.72      | 122.46   |
| 6   | O8    | 92   | ALA  | CA-C-N | -7.06 | 113.26      | 123.00   |
| 6   | O8    | 92   | ALA  | C-N-CA | -7.06 | 113.26      | 123.00   |
| 18  | B     | 1286 | ALA  | CA-C-N | -7.06 | 112.25      | 122.06   |
| 18  | B     | 1286 | ALA  | C-N-CA | -7.06 | 112.25      | 122.06   |
| 21  | H16   | 321  | SER  | O-C-N  | -7.06 | 113.20      | 122.59   |
| 5   | P8    | 648  | LEU  | O-C-N  | 7.06  | 130.20      | 122.15   |
| 10  | C24   | 640  | GLN  | O-C-N  | 7.06  | 129.34      | 122.07   |
| 21  | H8    | 321  | SER  | O-C-N  | -7.05 | 113.21      | 122.59   |
| 10  | C32   | 1084 | LYS  | O-C-N  | -7.05 | 113.21      | 122.59   |
| 1   | R     | 1198 | GLU  | CA-C-N | -7.05 | 111.28      | 120.44   |
| 1   | R     | 1198 | GLU  | C-N-CA | -7.05 | 111.28      | 120.44   |
| 10  | C32   | 454  | SER  | CA-C-N | 7.05  | 132.88      | 122.10   |
| 10  | C32   | 454  | SER  | C-N-CA | 7.05  | 132.88      | 122.10   |
| 1   | R     | 1202 | ARG  | CA-C-N | -7.04 | 110.86      | 120.44   |
| 1   | R     | 1202 | ARG  | C-N-CA | -7.04 | 110.86      | 120.44   |
| 10  | C     | 1084 | LYS  | O-C-N  | -7.04 | 113.22      | 122.59   |
| 18  | B8    | 1286 | ALA  | CA-C-N | -7.04 | 112.28      | 122.06   |
| 18  | B8    | 1286 | ALA  | C-N-CA | -7.04 | 112.28      | 122.06   |
| 17  | F8    | 78   | SER  | O-C-N  | -7.04 | 113.23      | 122.59   |
| 17  | F     | 78   | SER  | O-C-N  | -7.04 | 113.23      | 122.59   |
| 1   | R8    | 1202 | ARG  | CA-C-N | -7.03 | 110.88      | 120.44   |
| 1   | R8    | 1202 | ARG  | C-N-CA | -7.03 | 110.88      | 120.44   |
| 10  | C24   | 774  | GLY  | O-C-N  | -7.03 | 115.35      | 122.17   |
| 21  | H     | 321  | SER  | O-C-N  | -7.03 | 113.24      | 122.59   |
| 18  | B8    | 1673 | ARG  | CA-C-N | -7.03 | 111.30      | 120.44   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B8    | 1673 | ARG  | C-N-CA | -7.03 | 111.30      | 120.44   |
| 6   | O16   | 92   | ALA  | CA-C-N | -7.03 | 113.30      | 123.00   |
| 6   | O16   | 92   | ALA  | C-N-CA | -7.03 | 113.30      | 123.00   |
| 18  | B8    | 1114 | CYS  | CA-C-N | 7.03  | 134.62      | 121.97   |
| 18  | B8    | 1114 | CYS  | C-N-CA | 7.03  | 134.62      | 121.97   |
| 21  | H24   | 321  | SER  | O-C-N  | -7.03 | 113.24      | 122.59   |
| 7   | Q16   | 271  | ALA  | O-C-N  | -7.03 | 113.25      | 122.59   |
| 10  | C     | 774  | GLY  | O-C-N  | -7.03 | 115.36      | 122.17   |
| 10  | C8    | 422  | THR  | CA-C-N | -7.02 | 111.54      | 121.72   |
| 10  | C8    | 422  | THR  | C-N-CA | -7.02 | 111.54      | 121.72   |
| 10  | C     | 422  | THR  | CA-C-N | -7.02 | 111.54      | 121.72   |
| 10  | C     | 422  | THR  | C-N-CA | -7.02 | 111.54      | 121.72   |
| 6   | O     | 92   | ALA  | CA-C-N | -7.02 | 113.31      | 123.00   |
| 6   | O     | 92   | ALA  | C-N-CA | -7.02 | 113.31      | 123.00   |
| 5   | P16   | 648  | LEU  | O-C-N  | 7.02  | 130.15      | 122.15   |
| 9   | K     | 729  | VAL  | O-C-N  | -7.02 | 113.80      | 122.57   |
| 20  | E     | 39   | SER  | O-C-N  | -7.02 | 113.26      | 122.59   |
| 1   | R16   | 1202 | ARG  | CA-C-N | -7.01 | 110.90      | 120.44   |
| 1   | R16   | 1202 | ARG  | C-N-CA | -7.01 | 110.90      | 120.44   |
| 18  | B     | 1359 | GLU  | CA-C-N | 7.01  | 134.93      | 121.54   |
| 18  | B     | 1359 | GLU  | C-N-CA | 7.01  | 134.93      | 121.54   |
| 7   | Q8    | 271  | ALA  | O-C-N  | -7.01 | 113.27      | 122.59   |
| 10  | C16   | 411  | ASP  | O-C-N  | 7.01  | 129.55      | 122.12   |
| 18  | B8    | 975  | ASP  | O-C-N  | -7.01 | 112.79      | 122.46   |
| 9   | K8    | 641  | THR  | O-C-N  | -7.00 | 114.40      | 123.02   |
| 17  | F16   | 78   | SER  | O-C-N  | -7.00 | 113.27      | 122.59   |
| 17  | F24   | 78   | SER  | O-C-N  | -7.00 | 113.28      | 122.59   |
| 10  | C32   | 774  | GLY  | O-C-N  | -7.00 | 115.38      | 122.17   |
| 20  | E8    | 39   | SER  | O-C-N  | -7.00 | 113.28      | 122.59   |
| 15  | J     | 684  | ASP  | CA-C-N | -7.00 | 107.70      | 121.41   |
| 15  | J     | 684  | ASP  | C-N-CA | -7.00 | 107.70      | 121.41   |
| 18  | B8    | 1359 | GLU  | CA-C-N | 7.00  | 134.90      | 121.54   |
| 18  | B8    | 1359 | GLU  | C-N-CA | 7.00  | 134.90      | 121.54   |
| 10  | C24   | 411  | ASP  | O-C-N  | 7.00  | 129.53      | 122.12   |
| 10  | C8    | 411  | ASP  | O-C-N  | 6.99  | 129.53      | 122.12   |
| 9   | K8    | 729  | VAL  | O-C-N  | -6.99 | 113.83      | 122.57   |
| 7   | Q     | 271  | ALA  | O-C-N  | -6.98 | 113.30      | 122.59   |
| 10  | C16   | 408  | GLU  | O-C-N  | 6.98  | 129.52      | 122.12   |
| 10  | C16   | 640  | GLN  | O-C-N  | 6.98  | 129.26      | 122.07   |
| 10  | C16   | 774  | GLY  | O-C-N  | -6.97 | 115.41      | 122.17   |
| 10  | C32   | 411  | ASP  | O-C-N  | 6.97  | 129.51      | 122.12   |
| 10  | C32   | 328  | HIS  | O-C-N  | -6.97 | 114.73      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 641  | THR  | O-C-N  | -6.97 | 114.45      | 123.02   |
| 10  | C24   | 665  | ALA  | O-C-N  | 6.97  | 130.10      | 122.15   |
| 2   | M     | 327  | SER  | O-C-N  | -6.97 | 114.70      | 123.06   |
| 1   | R16   | 1246 | LYS  | CA-C-N | -6.97 | 113.20      | 120.38   |
| 1   | R16   | 1246 | LYS  | C-N-CA | -6.97 | 113.20      | 120.38   |
| 10  | C16   | 422  | THR  | CA-C-N | -6.97 | 111.62      | 121.72   |
| 10  | C16   | 422  | THR  | C-N-CA | -6.97 | 111.62      | 121.72   |
| 10  | C8    | 328  | HIS  | O-C-N  | -6.97 | 114.73      | 122.12   |
| 18  | B     | 1114 | CYS  | CA-C-N | 6.97  | 134.51      | 121.97   |
| 18  | B     | 1114 | CYS  | C-N-CA | 6.97  | 134.51      | 121.97   |
| 2   | M8    | 327  | SER  | O-C-N  | -6.96 | 114.70      | 123.06   |
| 18  | B     | 1270 | SER  | CA-C-N | 6.96  | 129.49      | 120.44   |
| 18  | B     | 1270 | SER  | C-N-CA | 6.96  | 129.49      | 120.44   |
| 10  | C     | 712  | LEU  | O-C-N  | -6.96 | 112.48      | 122.36   |
| 18  | B8    | 1788 | ILE  | CA-C-N | -6.96 | 108.25      | 121.54   |
| 18  | B8    | 1788 | ILE  | C-N-CA | -6.96 | 108.25      | 121.54   |
| 10  | C24   | 328  | HIS  | O-C-N  | -6.96 | 114.75      | 122.12   |
| 10  | C     | 328  | HIS  | O-C-N  | -6.96 | 114.75      | 122.12   |
| 10  | C32   | 422  | THR  | CA-C-N | -6.96 | 111.63      | 121.72   |
| 10  | C32   | 422  | THR  | C-N-CA | -6.96 | 111.63      | 121.72   |
| 10  | C     | 411  | ASP  | O-C-N  | 6.95  | 129.49      | 122.12   |
| 11  | A32   | 630  | ARG  | O-C-N  | 6.95  | 130.72      | 122.94   |
| 18  | B     | 1788 | ILE  | CA-C-N | -6.95 | 108.27      | 121.54   |
| 18  | B     | 1788 | ILE  | C-N-CA | -6.95 | 108.27      | 121.54   |
| 10  | C32   | 1061 | ASN  | CA-C-N | -6.95 | 104.85      | 121.80   |
| 10  | C32   | 1061 | ASN  | C-N-CA | -6.95 | 104.85      | 121.80   |
| 10  | C16   | 712  | LEU  | O-C-N  | -6.95 | 112.50      | 122.36   |
| 10  | C8    | 420  | TYR  | CA-C-N | 6.94  | 130.15      | 120.29   |
| 10  | C8    | 420  | TYR  | C-N-CA | 6.94  | 130.15      | 120.29   |
| 2   | M16   | 327  | SER  | O-C-N  | -6.94 | 114.73      | 123.06   |
| 18  | B     | 1666 | PRO  | O-C-N  | -6.94 | 114.77      | 123.10   |
| 10  | C32   | 408  | GLU  | O-C-N  | 6.94  | 129.48      | 122.12   |
| 10  | C8    | 1703 | ILE  | O-C-N  | -6.94 | 115.09      | 121.89   |
| 20  | E8    | 499  | PRO  | O-C-N  | 6.94  | 124.41      | 121.15   |
| 10  | C24   | 1084 | LYS  | O-C-N  | -6.94 | 113.36      | 122.59   |
| 11  | A40   | 630  | ARG  | O-C-N  | 6.93  | 130.71      | 122.94   |
| 10  | C     | 420  | TYR  | CA-C-N | 6.93  | 130.14      | 120.29   |
| 10  | C     | 420  | TYR  | C-N-CA | 6.93  | 130.14      | 120.29   |
| 9   | K     | 967  | ASP  | CA-C-N | 6.93  | 130.85      | 120.31   |
| 9   | K     | 967  | ASP  | C-N-CA | 6.93  | 130.85      | 120.31   |
| 10  | C24   | 422  | THR  | CA-C-N | -6.93 | 111.67      | 121.72   |
| 10  | C24   | 422  | THR  | C-N-CA | -6.93 | 111.67      | 121.72   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C     | 1703 | ILE  | O-C-N  | -6.93 | 115.10      | 121.89   |
| 18  | B8    | 975  | ASP  | CA-C-N | -6.93 | 111.96      | 122.21   |
| 18  | B8    | 975  | ASP  | C-N-CA | -6.93 | 111.96      | 122.21   |
| 10  | C16   | 420  | TYR  | CA-C-N | 6.92  | 130.12      | 120.29   |
| 10  | C16   | 420  | TYR  | C-N-CA | 6.92  | 130.12      | 120.29   |
| 10  | C     | 1061 | ASN  | CA-C-N | -6.92 | 104.90      | 121.80   |
| 10  | C     | 1061 | ASN  | C-N-CA | -6.92 | 104.90      | 121.80   |
| 10  | C8    | 640  | GLN  | O-C-N  | 6.92  | 129.20      | 122.07   |
| 10  | C32   | 420  | TYR  | CA-C-N | 6.92  | 130.11      | 120.29   |
| 10  | C32   | 420  | TYR  | C-N-CA | 6.92  | 130.11      | 120.29   |
| 10  | C24   | 712  | LEU  | O-C-N  | -6.92 | 112.54      | 122.36   |
| 10  | C8    | 1061 | ASN  | CA-C-N | -6.92 | 104.92      | 121.80   |
| 10  | C8    | 1061 | ASN  | C-N-CA | -6.92 | 104.92      | 121.80   |
| 12  | A48   | 630  | ARG  | O-C-N  | 6.92  | 130.69      | 122.94   |
| 10  | C32   | 1284 | ASP  | O-C-N  | 6.92  | 130.03      | 122.15   |
| 10  | C16   | 1061 | ASN  | CA-C-N | -6.91 | 104.93      | 121.80   |
| 10  | C16   | 1061 | ASN  | C-N-CA | -6.91 | 104.93      | 121.80   |
| 14  | W     | 608  | SER  | O-C-N  | 6.91  | 131.31      | 122.39   |
| 18  | B8    | 1666 | PRO  | O-C-N  | -6.91 | 114.80      | 123.10   |
| 10  | C32   | 712  | LEU  | O-C-N  | -6.91 | 112.54      | 122.36   |
| 9   | K8    | 967  | ASP  | CA-C-N | 6.91  | 130.81      | 120.31   |
| 9   | K8    | 967  | ASP  | C-N-CA | 6.91  | 130.81      | 120.31   |
| 10  | C8    | 1126 | ASP  | O-C-N  | -6.91 | 113.40      | 122.59   |
| 11  | A16   | 630  | ARG  | O-C-N  | 6.91  | 130.68      | 122.94   |
| 10  | C32   | 1703 | ILE  | O-C-N  | -6.91 | 115.12      | 121.89   |
| 1   | R8    | 1246 | LYS  | CA-C-N | -6.91 | 113.26      | 120.38   |
| 1   | R8    | 1246 | LYS  | C-N-CA | -6.91 | 113.26      | 120.38   |
| 9   | K8    | 594  | GLY  | O-C-N  | 6.91  | 128.82      | 122.19   |
| 10  | C     | 1284 | ASP  | O-C-N  | 6.91  | 130.03      | 122.15   |
| 12  | A48   | 631  | GLU  | O-C-N  | -6.91 | 113.82      | 123.01   |
| 10  | C24   | 420  | TYR  | CA-C-N | 6.90  | 130.09      | 120.29   |
| 10  | C24   | 420  | TYR  | C-N-CA | 6.90  | 130.09      | 120.29   |
| 13  | V     | 889  | SER  | O-C-N  | -6.90 | 114.33      | 122.89   |
| 10  | C8    | 712  | LEU  | O-C-N  | -6.90 | 112.56      | 122.36   |
| 6   | O     | 180  | GLY  | CA-C-N | 6.90  | 134.72      | 121.54   |
| 6   | O     | 180  | GLY  | C-N-CA | 6.90  | 134.72      | 121.54   |
| 6   | O8    | 180  | GLY  | CA-C-N | 6.90  | 134.72      | 121.54   |
| 6   | O8    | 180  | GLY  | C-N-CA | 6.90  | 134.72      | 121.54   |
| 10  | C16   | 328  | HIS  | O-C-N  | -6.90 | 114.81      | 122.12   |
| 18  | B8    | 194  | ASN  | CA-C-N | -6.90 | 113.48      | 123.00   |
| 18  | B8    | 194  | ASN  | C-N-CA | -6.90 | 113.48      | 123.00   |
| 10  | C16   | 1703 | ILE  | O-C-N  | -6.90 | 115.13      | 121.89   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 1061 | ASN  | CA-C-N | -6.90 | 104.97      | 121.80   |
| 10  | C24   | 1061 | ASN  | C-N-CA | -6.90 | 104.97      | 121.80   |
| 6   | O16   | 180  | GLY  | CA-C-N | 6.89  | 134.71      | 121.54   |
| 6   | O16   | 180  | GLY  | C-N-CA | 6.89  | 134.71      | 121.54   |
| 10  | C     | 640  | GLN  | O-C-N  | 6.89  | 129.17      | 122.07   |
| 18  | B8    | 1270 | SER  | CA-C-N | 6.89  | 129.40      | 120.44   |
| 18  | B8    | 1270 | SER  | C-N-CA | 6.89  | 129.40      | 120.44   |
| 18  | B     | 975  | ASP  | CA-C-N | -6.89 | 112.01      | 122.21   |
| 18  | B     | 975  | ASP  | C-N-CA | -6.89 | 112.01      | 122.21   |
| 18  | B     | 1284 | ASN  | O-C-N  | -6.89 | 113.17      | 122.68   |
| 10  | C8    | 1284 | ASP  | O-C-N  | 6.89  | 130.00      | 122.15   |
| 1   | R     | 1246 | LYS  | CA-C-N | -6.88 | 113.29      | 120.38   |
| 1   | R     | 1246 | LYS  | C-N-CA | -6.88 | 113.29      | 120.38   |
| 10  | C8    | 408  | GLU  | O-C-N  | 6.88  | 129.42      | 122.12   |
| 20  | E     | 499  | PRO  | O-C-N  | 6.88  | 124.39      | 121.15   |
| 10  | C24   | 1776 | SER  | O-C-N  | -6.88 | 113.01      | 122.30   |
| 10  | C16   | 1070 | PRO  | CA-C-N | 6.88  | 134.69      | 121.54   |
| 10  | C16   | 1070 | PRO  | C-N-CA | 6.88  | 134.69      | 121.54   |
| 11  | A24   | 159  | LYS  | CA-C-N | -6.88 | 109.31      | 121.70   |
| 11  | A24   | 159  | LYS  | C-N-CA | -6.88 | 109.31      | 121.70   |
| 10  | C32   | 1776 | SER  | O-C-N  | -6.88 | 113.01      | 122.30   |
| 10  | C24   | 1284 | ASP  | O-C-N  | 6.88  | 129.99      | 122.15   |
| 10  | C16   | 1284 | ASP  | O-C-N  | 6.88  | 129.99      | 122.15   |
| 11  | A24   | 630  | ARG  | O-C-N  | 6.88  | 130.65      | 122.94   |
| 10  | C24   | 408  | GLU  | O-C-N  | 6.88  | 129.41      | 122.12   |
| 18  | B8    | 823  | GLU  | CA-C-N | 6.88  | 127.16      | 119.32   |
| 18  | B8    | 823  | GLU  | C-N-CA | 6.88  | 127.16      | 119.32   |
| 10  | C24   | 1703 | ILE  | O-C-N  | -6.88 | 115.15      | 121.89   |
| 10  | C24   | 1070 | PRO  | CA-C-N | 6.87  | 134.66      | 121.54   |
| 10  | C24   | 1070 | PRO  | C-N-CA | 6.87  | 134.66      | 121.54   |
| 18  | B8    | 499  | ILE  | O-C-N  | -6.87 | 115.19      | 122.68   |
| 10  | C32   | 1507 | LEU  | CA-C-N | 6.87  | 134.67      | 121.54   |
| 10  | C32   | 1507 | LEU  | C-N-CA | 6.87  | 134.67      | 121.54   |
| 19  | 48    | 52   | SER  | O-C-N  | -6.87 | 113.45      | 122.59   |
| 10  | C32   | 1070 | PRO  | CA-C-N | 6.87  | 134.66      | 121.54   |
| 10  | C32   | 1070 | PRO  | C-N-CA | 6.87  | 134.66      | 121.54   |
| 10  | C16   | 1507 | LEU  | CA-C-N | 6.87  | 134.65      | 121.54   |
| 10  | C16   | 1507 | LEU  | C-N-CA | 6.87  | 134.65      | 121.54   |
| 18  | B     | 194  | ASN  | CA-C-N | -6.86 | 113.53      | 123.00   |
| 18  | B     | 194  | ASN  | C-N-CA | -6.86 | 113.53      | 123.00   |
| 19  | 4     | 52   | SER  | O-C-N  | -6.86 | 113.46      | 122.59   |
| 20  | E     | 428  | GLY  | CA-C-N | 6.86  | 128.42      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 20  | E     | 428  | GLY  | C-N-CA | 6.86  | 128.42      | 119.84   |
| 1   | R16   | 1293 | CYS  | O-C-N  | -6.86 | 115.04      | 121.35   |
| 10  | C     | 408  | GLU  | O-C-N  | 6.86  | 129.39      | 122.12   |
| 18  | B8    | 156  | ALA  | CA-C-N | 6.86  | 126.66      | 119.05   |
| 18  | B8    | 156  | ALA  | C-N-CA | 6.86  | 126.66      | 119.05   |
| 20  | E     | 446  | PRO  | O-C-N  | -6.86 | 113.39      | 122.64   |
| 10  | C16   | 538  | PHE  | O-C-N  | -6.85 | 114.59      | 123.02   |
| 20  | E8    | 446  | PRO  | O-C-N  | -6.85 | 113.39      | 122.64   |
| 18  | B8    | 1284 | ASN  | O-C-N  | -6.85 | 113.22      | 122.68   |
| 10  | C24   | 1507 | LEU  | CA-C-N | 6.85  | 134.62      | 121.54   |
| 10  | C24   | 1507 | LEU  | C-N-CA | 6.85  | 134.62      | 121.54   |
| 10  | C     | 727  | THR  | CA-C-N | -6.85 | 110.88      | 121.02   |
| 10  | C     | 727  | THR  | C-N-CA | -6.85 | 110.88      | 121.02   |
| 10  | C     | 1126 | ASP  | O-C-N  | -6.85 | 113.48      | 122.59   |
| 15  | J     | 638  | ASP  | CA-C-N | 6.84  | 129.34      | 120.44   |
| 15  | J     | 638  | ASP  | C-N-CA | 6.84  | 129.34      | 120.44   |
| 10  | C32   | 1126 | ASP  | O-C-N  | -6.84 | 113.49      | 122.59   |
| 18  | B     | 1635 | GLY  | O-C-N  | -6.84 | 115.02      | 122.54   |
| 12  | A48   | 159  | LYS  | CA-C-N | -6.84 | 109.38      | 121.70   |
| 12  | A48   | 159  | LYS  | C-N-CA | -6.84 | 109.38      | 121.70   |
| 10  | C8    | 1776 | SER  | O-C-N  | -6.84 | 113.07      | 122.30   |
| 11  | A32   | 631  | GLU  | O-C-N  | -6.84 | 113.91      | 123.01   |
| 10  | C32   | 538  | PHE  | O-C-N  | -6.84 | 114.61      | 123.02   |
| 9   | K     | 594  | GLY  | O-C-N  | 6.84  | 128.75      | 122.19   |
| 10  | C     | 1070 | PRO  | CA-C-N | 6.84  | 134.60      | 121.54   |
| 10  | C     | 1070 | PRO  | C-N-CA | 6.84  | 134.60      | 121.54   |
| 20  | E8    | 428  | GLY  | CA-C-N | 6.83  | 128.38      | 119.84   |
| 20  | E8    | 428  | GLY  | C-N-CA | 6.83  | 128.38      | 119.84   |
| 11  | A40   | 159  | LYS  | CA-C-N | -6.83 | 109.40      | 121.70   |
| 11  | A40   | 159  | LYS  | C-N-CA | -6.83 | 109.40      | 121.70   |
| 18  | B8    | 1132 | TRP  | O-C-N  | -6.83 | 113.50      | 122.59   |
| 12  | A     | 630  | ARG  | O-C-N  | 6.83  | 130.59      | 122.94   |
| 1   | R8    | 1293 | CYS  | O-C-N  | -6.83 | 115.07      | 121.35   |
| 10  | C16   | 727  | THR  | CA-C-N | -6.83 | 110.91      | 121.02   |
| 10  | C16   | 727  | THR  | C-N-CA | -6.83 | 110.91      | 121.02   |
| 12  | A     | 631  | GLU  | O-C-N  | -6.83 | 113.93      | 123.01   |
| 10  | C16   | 1126 | ASP  | O-C-N  | -6.83 | 113.51      | 122.59   |
| 10  | C24   | 727  | THR  | CA-C-N | -6.83 | 110.92      | 121.02   |
| 10  | C24   | 727  | THR  | C-N-CA | -6.83 | 110.92      | 121.02   |
| 18  | B     | 1132 | TRP  | O-C-N  | -6.83 | 113.51      | 122.59   |
| 10  | C     | 1507 | LEU  | CA-C-N | 6.82  | 134.57      | 121.54   |
| 10  | C     | 1507 | LEU  | C-N-CA | 6.82  | 134.57      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 538  | PHE  | O-C-N  | -6.82 | 114.63      | 123.02   |
| 12  | A     | 159  | LYS  | CA-C-N | -6.82 | 109.42      | 121.70   |
| 12  | A     | 159  | LYS  | C-N-CA | -6.82 | 109.42      | 121.70   |
| 18  | B     | 823  | GLU  | CA-C-N | 6.82  | 127.09      | 119.32   |
| 18  | B     | 823  | GLU  | C-N-CA | 6.82  | 127.09      | 119.32   |
| 11  | A24   | 631  | GLU  | O-C-N  | -6.81 | 113.95      | 123.01   |
| 10  | C24   | 1126 | ASP  | O-C-N  | -6.81 | 113.53      | 122.59   |
| 10  | C24   | 1596 | GLU  | O-C-N  | -6.81 | 115.30      | 123.13   |
| 10  | C8    | 1070 | PRO  | CA-C-N | 6.81  | 134.55      | 121.54   |
| 10  | C8    | 1070 | PRO  | C-N-CA | 6.81  | 134.55      | 121.54   |
| 10  | C8    | 1596 | GLU  | O-C-N  | -6.81 | 115.30      | 123.13   |
| 18  | B8    | 1637 | VAL  | O-C-N  | -6.81 | 115.47      | 123.03   |
| 19  | 48    | 68   | GLY  | O-C-N  | -6.81 | 113.85      | 122.70   |
| 1   | R     | 1293 | CYS  | O-C-N  | -6.81 | 115.09      | 121.35   |
| 2   | M     | 758  | GLU  | CA-C-N | 6.81  | 134.54      | 121.54   |
| 2   | M     | 758  | GLU  | C-N-CA | 6.81  | 134.54      | 121.54   |
| 15  | J     | 687  | SER  | CA-C-N | 6.81  | 128.35      | 119.84   |
| 15  | J     | 687  | SER  | C-N-CA | 6.81  | 128.35      | 119.84   |
| 10  | C8    | 1507 | LEU  | CA-C-N | 6.81  | 134.54      | 121.54   |
| 10  | C8    | 1507 | LEU  | C-N-CA | 6.81  | 134.54      | 121.54   |
| 10  | C     | 1776 | SER  | O-C-N  | -6.80 | 113.12      | 122.30   |
| 10  | C32   | 727  | THR  | CA-C-N | -6.80 | 110.95      | 121.02   |
| 10  | C32   | 727  | THR  | C-N-CA | -6.80 | 110.95      | 121.02   |
| 10  | C     | 538  | PHE  | O-C-N  | -6.80 | 114.66      | 123.02   |
| 10  | C16   | 1776 | SER  | O-C-N  | -6.80 | 113.12      | 122.30   |
| 16  | A8    | 159  | LYS  | CA-C-N | -6.79 | 109.47      | 121.70   |
| 16  | A8    | 159  | LYS  | C-N-CA | -6.79 | 109.47      | 121.70   |
| 10  | C32   | 1596 | GLU  | O-C-N  | -6.79 | 115.32      | 123.13   |
| 19  | 4     | 68   | GLY  | O-C-N  | -6.79 | 113.87      | 122.70   |
| 2   | M8    | 758  | GLU  | CA-C-N | 6.78  | 134.50      | 121.54   |
| 2   | M8    | 758  | GLU  | C-N-CA | 6.78  | 134.50      | 121.54   |
| 11  | A40   | 631  | GLU  | O-C-N  | -6.78 | 113.99      | 123.01   |
| 10  | C     | 1621 | LYS  | O-C-N  | -6.78 | 114.31      | 122.11   |
| 18  | B     | 156  | ALA  | CA-C-N | 6.78  | 126.57      | 119.05   |
| 18  | B     | 156  | ALA  | C-N-CA | 6.78  | 126.57      | 119.05   |
| 10  | C16   | 1596 | GLU  | O-C-N  | -6.78 | 115.34      | 123.13   |
| 11  | A16   | 631  | GLU  | O-C-N  | -6.77 | 114.00      | 123.01   |
| 18  | B8    | 680  | SER  | CA-C-N | 6.77  | 134.68      | 121.41   |
| 18  | B8    | 680  | SER  | C-N-CA | 6.77  | 134.68      | 121.41   |
| 10  | C     | 1596 | GLU  | O-C-N  | -6.77 | 115.35      | 123.13   |
| 10  | C32   | 1621 | LYS  | O-C-N  | -6.76 | 114.33      | 122.11   |
| 1   | R16   | 1203 | SER  | O-C-N  | -6.76 | 114.79      | 122.09   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 499  | ILE  | O-C-N  | -6.76 | 115.31      | 122.68   |
| 18  | B     | 1791 | VAL  | O-C-N  | -6.76 | 114.12      | 122.57   |
| 18  | B     | 1637 | VAL  | O-C-N  | -6.76 | 115.53      | 123.03   |
| 18  | B8    | 1635 | GLY  | O-C-N  | -6.76 | 115.10      | 122.54   |
| 9   | K8    | 1048 | GLN  | O-C-N  | -6.76 | 113.60      | 122.59   |
| 18  | B     | 680  | SER  | CA-C-N | 6.75  | 134.65      | 121.41   |
| 18  | B     | 680  | SER  | C-N-CA | 6.75  | 134.65      | 121.41   |
| 2   | M16   | 758  | GLU  | CA-C-N | 6.75  | 134.43      | 121.54   |
| 2   | M16   | 758  | GLU  | C-N-CA | 6.75  | 134.43      | 121.54   |
| 10  | C24   | 538  | PHE  | O-C-N  | -6.75 | 114.72      | 123.02   |
| 13  | V     | 872  | ASP  | O-C-N  | -6.75 | 110.19      | 122.34   |
| 18  | B     | 1943 | HIS  | CA-C-N | 6.75  | 130.00      | 120.28   |
| 18  | B     | 1943 | HIS  | C-N-CA | 6.75  | 130.00      | 120.28   |
| 10  | C     | 1127 | THR  | O-C-N  | -6.74 | 113.63      | 122.39   |
| 10  | C8    | 1621 | LYS  | O-C-N  | -6.74 | 114.36      | 122.11   |
| 10  | C24   | 378  | GLU  | CA-C-N | 6.74  | 129.31      | 120.28   |
| 10  | C24   | 378  | GLU  | C-N-CA | 6.74  | 129.31      | 120.28   |
| 18  | B8    | 1791 | VAL  | O-C-N  | -6.74 | 114.15      | 122.57   |
| 9   | K     | 1048 | GLN  | O-C-N  | -6.74 | 113.63      | 122.59   |
| 10  | C16   | 1430 | ARG  | O-C-N  | 6.73  | 129.26      | 122.12   |
| 1   | R8    | 1209 | GLY  | CA-C-N | 6.73  | 134.39      | 121.54   |
| 1   | R8    | 1209 | GLY  | C-N-CA | 6.73  | 134.39      | 121.54   |
| 10  | C8    | 468  | GLU  | CA-C-N | 6.72  | 131.69      | 122.34   |
| 10  | C8    | 468  | GLU  | C-N-CA | 6.72  | 131.69      | 122.34   |
| 10  | C     | 468  | GLU  | CA-C-N | 6.72  | 131.68      | 122.34   |
| 10  | C     | 468  | GLU  | C-N-CA | 6.72  | 131.68      | 122.34   |
| 10  | C32   | 1430 | ARG  | O-C-N  | 6.72  | 129.24      | 122.12   |
| 1   | R     | 1209 | GLY  | CA-C-N | 6.72  | 134.37      | 121.54   |
| 1   | R     | 1209 | GLY  | C-N-CA | 6.72  | 134.37      | 121.54   |
| 10  | C16   | 468  | GLU  | CA-C-N | 6.71  | 131.67      | 122.34   |
| 10  | C16   | 468  | GLU  | C-N-CA | 6.71  | 131.67      | 122.34   |
| 18  | B8    | 510  | GLN  | O-C-N  | -6.71 | 114.09      | 122.35   |
| 1   | R8    | 1203 | SER  | O-C-N  | -6.71 | 114.84      | 122.09   |
| 10  | C24   | 1127 | THR  | O-C-N  | -6.71 | 113.66      | 122.39   |
| 1   | R     | 1203 | SER  | O-C-N  | -6.71 | 114.84      | 122.09   |
| 10  | C16   | 1621 | LYS  | O-C-N  | -6.71 | 114.39      | 122.11   |
| 9   | K     | 1280 | PHE  | CA-C-N | 6.70  | 133.56      | 121.97   |
| 9   | K     | 1280 | PHE  | C-N-CA | 6.70  | 133.56      | 121.97   |
| 18  | B8    | 1943 | HIS  | CA-C-N | 6.70  | 129.93      | 120.28   |
| 18  | B8    | 1943 | HIS  | C-N-CA | 6.70  | 129.93      | 120.28   |
| 10  | C32   | 378  | GLU  | CA-C-N | 6.70  | 129.26      | 120.28   |
| 10  | C32   | 378  | GLU  | C-N-CA | 6.70  | 129.26      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 468  | GLU  | CA-C-N | 6.70  | 131.65      | 122.34   |
| 10  | C24   | 468  | GLU  | C-N-CA | 6.70  | 131.65      | 122.34   |
| 10  | C32   | 468  | GLU  | CA-C-N | 6.70  | 131.65      | 122.34   |
| 10  | C32   | 468  | GLU  | C-N-CA | 6.70  | 131.65      | 122.34   |
| 10  | C8    | 1127 | THR  | O-C-N  | -6.70 | 113.69      | 122.39   |
| 21  | H24   | 181  | MET  | CA-C-N | 6.69  | 130.86      | 120.75   |
| 21  | H24   | 181  | MET  | C-N-CA | 6.69  | 130.86      | 120.75   |
| 10  | C24   | 1430 | ARG  | O-C-N  | 6.69  | 129.21      | 122.12   |
| 9   | K8    | 1280 | PHE  | CA-C-N | 6.69  | 133.54      | 121.97   |
| 9   | K8    | 1280 | PHE  | C-N-CA | 6.69  | 133.54      | 121.97   |
| 18  | B8    | 161  | SER  | CA-C-N | 6.69  | 130.15      | 120.38   |
| 18  | B8    | 161  | SER  | C-N-CA | 6.69  | 130.15      | 120.38   |
| 1   | R16   | 1209 | GLY  | CA-C-N | 6.69  | 134.31      | 121.54   |
| 1   | R16   | 1209 | GLY  | C-N-CA | 6.69  | 134.31      | 121.54   |
| 18  | B     | 510  | GLN  | O-C-N  | -6.69 | 114.13      | 122.35   |
| 10  | C     | 378  | GLU  | CA-C-N | 6.68  | 129.24      | 120.28   |
| 10  | C     | 378  | GLU  | C-N-CA | 6.68  | 129.24      | 120.28   |
| 18  | B8    | 986  | ALA  | CA-C-N | 6.68  | 134.31      | 121.54   |
| 18  | B8    | 986  | ALA  | C-N-CA | 6.68  | 134.31      | 121.54   |
| 19  | 48    | 62   | ASN  | CA-C-N | 6.68  | 134.51      | 121.41   |
| 19  | 48    | 62   | ASN  | C-N-CA | 6.68  | 134.51      | 121.41   |
| 21  | H     | 181  | MET  | CA-C-N | 6.68  | 130.84      | 120.75   |
| 21  | H     | 181  | MET  | C-N-CA | 6.68  | 130.84      | 120.75   |
| 19  | 4     | 62   | ASN  | CA-C-N | 6.68  | 134.50      | 121.41   |
| 19  | 4     | 62   | ASN  | C-N-CA | 6.68  | 134.50      | 121.41   |
| 18  | B8    | 1786 | PRO  | CA-C-N | -6.68 | 108.78      | 121.54   |
| 18  | B8    | 1786 | PRO  | C-N-CA | -6.68 | 108.78      | 121.54   |
| 20  | E     | 204  | SER  | CA-C-N | -6.68 | 113.16      | 120.44   |
| 20  | E     | 204  | SER  | C-N-CA | -6.68 | 113.16      | 120.44   |
| 18  | B     | 161  | SER  | CA-C-N | 6.67  | 130.12      | 120.38   |
| 18  | B     | 161  | SER  | C-N-CA | 6.67  | 130.12      | 120.38   |
| 10  | C32   | 421  | ARG  | O-C-N  | -6.67 | 114.55      | 122.15   |
| 10  | C16   | 1127 | THR  | O-C-N  | -6.67 | 113.72      | 122.39   |
| 20  | E8    | 204  | SER  | CA-C-N | -6.67 | 113.17      | 120.44   |
| 20  | E8    | 204  | SER  | C-N-CA | -6.67 | 113.17      | 120.44   |
| 7   | Q8    | 298  | SER  | CA-C-N | 6.67  | 134.28      | 121.54   |
| 7   | Q8    | 298  | SER  | C-N-CA | 6.67  | 134.28      | 121.54   |
| 18  | B     | 1707 | TRP  | CA-C-N | 6.67  | 129.11      | 120.44   |
| 18  | B     | 1707 | TRP  | C-N-CA | 6.67  | 129.11      | 120.44   |
| 10  | C32   | 1127 | THR  | O-C-N  | -6.67 | 113.72      | 122.39   |
| 2   | M     | 815  | SER  | O-C-N  | -6.67 | 115.46      | 123.13   |
| 10  | C16   | 421  | ARG  | O-C-N  | -6.67 | 114.55      | 122.15   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 21  | H16   | 181  | MET  | CA-C-N | 6.67  | 130.82      | 120.75   |
| 21  | H16   | 181  | MET  | C-N-CA | 6.67  | 130.82      | 120.75   |
| 9   | K8    | 1240 | SER  | O-C-N  | -6.67 | 113.73      | 122.59   |
| 10  | C24   | 1783 | TYR  | O-C-N  | -6.66 | 114.14      | 122.20   |
| 10  | C8    | 421  | ARG  | O-C-N  | -6.66 | 114.56      | 122.15   |
| 10  | C8    | 1430 | ARG  | O-C-N  | 6.66  | 129.18      | 122.12   |
| 18  | B     | 1786 | PRO  | CA-C-N | -6.66 | 108.82      | 121.54   |
| 18  | B     | 1786 | PRO  | C-N-CA | -6.66 | 108.82      | 121.54   |
| 10  | C16   | 378  | GLU  | CA-C-N | 6.66  | 129.20      | 120.28   |
| 10  | C16   | 378  | GLU  | C-N-CA | 6.66  | 129.20      | 120.28   |
| 21  | H24   | 139  | ASP  | O-C-N  | 6.66  | 129.46      | 121.60   |
| 10  | C     | 1783 | TYR  | O-C-N  | -6.66 | 114.15      | 122.20   |
| 5   | P16   | 20   | GLU  | O-C-N  | -6.65 | 113.74      | 122.59   |
| 10  | C24   | 421  | ARG  | O-C-N  | -6.65 | 114.57      | 122.15   |
| 15  | J     | 723  | GLN  | O-C-N  | -6.65 | 114.09      | 122.27   |
| 2   | M16   | 815  | SER  | CA-C-N | 6.65  | 131.33      | 120.63   |
| 2   | M16   | 815  | SER  | C-N-CA | 6.65  | 131.33      | 120.63   |
| 10  | C8    | 1783 | TYR  | O-C-N  | -6.65 | 114.16      | 122.20   |
| 10  | C     | 1430 | ARG  | O-C-N  | 6.64  | 129.16      | 122.12   |
| 11  | A40   | 467  | SER  | O-C-N  | -6.64 | 114.45      | 122.22   |
| 2   | M     | 815  | SER  | CA-C-N | 6.64  | 131.32      | 120.63   |
| 2   | M     | 815  | SER  | C-N-CA | 6.64  | 131.32      | 120.63   |
| 7   | Q16   | 298  | SER  | CA-C-N | 6.64  | 134.22      | 121.54   |
| 7   | Q16   | 298  | SER  | C-N-CA | 6.64  | 134.22      | 121.54   |
| 11  | A24   | 467  | SER  | O-C-N  | -6.64 | 114.45      | 122.22   |
| 10  | C8    | 1506 | LYS  | CA-C-N | -6.64 | 110.63      | 122.32   |
| 10  | C8    | 1506 | LYS  | C-N-CA | -6.64 | 110.63      | 122.32   |
| 9   | K8    | 1269 | CYS  | CA-C-N | 6.64  | 132.09      | 121.34   |
| 9   | K8    | 1269 | CYS  | C-N-CA | 6.64  | 132.09      | 121.34   |
| 10  | C24   | 1621 | LYS  | O-C-N  | -6.63 | 114.48      | 122.11   |
| 10  | C     | 421  | ARG  | O-C-N  | -6.63 | 114.59      | 122.15   |
| 18  | B     | 986  | ALA  | CA-C-N | 6.63  | 134.21      | 121.54   |
| 18  | B     | 986  | ALA  | C-N-CA | 6.63  | 134.21      | 121.54   |
| 9   | K     | 1240 | SER  | O-C-N  | -6.63 | 113.77      | 122.59   |
| 14  | W     | 701  | LEU  | O-C-N  | -6.63 | 115.23      | 121.20   |
| 18  | B8    | 1707 | TRP  | CA-C-N | 6.63  | 129.06      | 120.44   |
| 18  | B8    | 1707 | TRP  | C-N-CA | 6.63  | 129.06      | 120.44   |
| 10  | C8    | 378  | GLU  | CA-C-N | 6.63  | 129.16      | 120.28   |
| 10  | C8    | 378  | GLU  | C-N-CA | 6.63  | 129.16      | 120.28   |
| 9   | K     | 1269 | CYS  | CA-C-N | 6.63  | 132.07      | 121.34   |
| 9   | K     | 1269 | CYS  | C-N-CA | 6.63  | 132.07      | 121.34   |
| 7   | Q     | 298  | SER  | CA-C-N | 6.62  | 134.19      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7   | Q     | 298  | SER  | C-N-CA | 6.62  | 134.19      | 121.54   |
| 2   | M8    | 815  | SER  | O-C-N  | -6.62 | 115.52      | 123.13   |
| 9   | K     | 937  | ILE  | O-C-N  | 6.62  | 128.65      | 121.83   |
| 9   | K8    | 937  | ILE  | O-C-N  | 6.62  | 128.65      | 121.83   |
| 21  | H24   | 373  | MET  | O-C-N  | 6.62  | 129.70      | 122.15   |
| 21  | H16   | 139  | ASP  | O-C-N  | 6.62  | 129.41      | 121.60   |
| 10  | C32   | 1783 | TYR  | O-C-N  | -6.62 | 114.19      | 122.20   |
| 9   | K8    | 989  | VAL  | O-C-N  | 6.62  | 128.29      | 121.87   |
| 2   | M16   | 815  | SER  | O-C-N  | -6.61 | 115.52      | 123.13   |
| 10  | C16   | 1783 | TYR  | O-C-N  | -6.61 | 114.20      | 122.20   |
| 14  | W     | 704  | THR  | CA-C-N | -6.61 | 110.68      | 122.32   |
| 14  | W     | 704  | THR  | C-N-CA | -6.61 | 110.68      | 122.32   |
| 2   | M8    | 815  | SER  | CA-C-N | 6.61  | 131.28      | 120.63   |
| 2   | M8    | 815  | SER  | C-N-CA | 6.61  | 131.28      | 120.63   |
| 5   | P8    | 20   | GLU  | O-C-N  | -6.61 | 113.80      | 122.59   |
| 21  | H8    | 139  | ASP  | O-C-N  | 6.61  | 129.40      | 121.60   |
| 5   | P     | 20   | GLU  | O-C-N  | -6.61 | 113.80      | 122.59   |
| 9   | K     | 989  | VAL  | O-C-N  | 6.61  | 128.28      | 121.87   |
| 14  | W     | 609  | THR  | O-C-N  | -6.61 | 115.69      | 121.31   |
| 14  | W     | 709  | LEU  | O-C-N  | -6.60 | 114.76      | 122.95   |
| 10  | C8    | 404  | ASP  | O-C-N  | 6.60  | 129.12      | 122.12   |
| 10  | C16   | 1506 | LYS  | CA-C-N | -6.60 | 110.70      | 122.32   |
| 10  | C16   | 1506 | LYS  | C-N-CA | -6.60 | 110.70      | 122.32   |
| 21  | H8    | 181  | MET  | CA-C-N | 6.60  | 130.71      | 120.75   |
| 21  | H8    | 181  | MET  | C-N-CA | 6.60  | 130.71      | 120.75   |
| 21  | H8    | 373  | MET  | O-C-N  | 6.60  | 129.67      | 122.15   |
| 9   | K8    | 913  | ARG  | O-C-N  | 6.60  | 129.11      | 122.12   |
| 10  | C32   | 1506 | LYS  | CA-C-N | -6.60 | 110.71      | 122.32   |
| 10  | C32   | 1506 | LYS  | C-N-CA | -6.60 | 110.71      | 122.32   |
| 10  | C16   | 881  | GLU  | O-C-N  | -6.59 | 114.91      | 123.02   |
| 10  | C24   | 881  | GLU  | O-C-N  | -6.59 | 114.91      | 123.02   |
| 10  | C     | 1506 | LYS  | CA-C-N | -6.59 | 110.72      | 122.32   |
| 10  | C     | 1506 | LYS  | C-N-CA | -6.59 | 110.72      | 122.32   |
| 9   | K8    | 1117 | LEU  | O-C-N  | -6.59 | 115.71      | 121.31   |
| 18  | B     | 614  | MET  | CA-C-N | 6.59  | 134.13      | 121.54   |
| 18  | B     | 614  | MET  | C-N-CA | 6.59  | 134.13      | 121.54   |
| 20  | E     | 207  | LEU  | CA-C-N | -6.59 | 110.11      | 121.97   |
| 20  | E     | 207  | LEU  | C-N-CA | -6.59 | 110.11      | 121.97   |
| 10  | C8    | 1064 | PHE  | CA-C-N | 6.58  | 134.11      | 121.54   |
| 10  | C8    | 1064 | PHE  | C-N-CA | 6.58  | 134.11      | 121.54   |
| 11  | A32   | 467  | SER  | O-C-N  | -6.58 | 114.52      | 122.22   |
| 12  | A     | 467  | SER  | O-C-N  | -6.58 | 114.52      | 122.22   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1771 | GLN  | O-C-N  | -6.58 | 113.39      | 122.46   |
| 21  | H     | 139  | ASP  | O-C-N  | 6.58  | 129.36      | 121.60   |
| 10  | C24   | 1506 | LYS  | CA-C-N | -6.57 | 110.75      | 122.32   |
| 10  | C24   | 1506 | LYS  | C-N-CA | -6.57 | 110.75      | 122.32   |
| 10  | C     | 104  | GLU  | O-C-N  | -6.57 | 112.62      | 122.28   |
| 19  | 48    | 187  | SER  | O-C-N  | -6.57 | 113.85      | 122.59   |
| 10  | C     | 626  | GLN  | O-C-N  | -6.57 | 113.79      | 122.33   |
| 10  | C32   | 881  | GLU  | O-C-N  | -6.57 | 114.94      | 123.02   |
| 15  | J     | 680  | LEU  | CA-C-N | -6.57 | 111.38      | 120.38   |
| 15  | J     | 680  | LEU  | C-N-CA | -6.57 | 111.38      | 120.38   |
| 9   | K     | 1117 | LEU  | O-C-N  | -6.57 | 115.73      | 121.31   |
| 3   | N     | 20   | ASP  | CA-C-N | 6.57  | 129.08      | 120.28   |
| 3   | N     | 20   | ASP  | C-N-CA | 6.57  | 129.08      | 120.28   |
| 9   | K     | 913  | ARG  | O-C-N  | 6.57  | 129.08      | 122.12   |
| 18  | B8    | 856  | LEU  | CA-C-N | 6.57  | 128.05      | 119.84   |
| 18  | B8    | 856  | LEU  | C-N-CA | 6.57  | 128.05      | 119.84   |
| 21  | H16   | 373  | MET  | O-C-N  | 6.57  | 129.63      | 122.15   |
| 8   | L     | 149  | SER  | CA-C-N | 6.56  | 124.38      | 120.24   |
| 8   | L     | 149  | SER  | C-N-CA | 6.56  | 124.38      | 120.24   |
| 10  | C16   | 404  | ASP  | O-C-N  | 6.56  | 129.08      | 122.12   |
| 10  | C16   | 626  | GLN  | O-C-N  | -6.56 | 113.80      | 122.33   |
| 18  | B8    | 1962 | PRO  | CA-C-N | 6.56  | 132.81      | 122.51   |
| 18  | B8    | 1962 | PRO  | C-N-CA | 6.56  | 132.81      | 122.51   |
| 20  | E8    | 207  | LEU  | CA-C-N | -6.56 | 110.16      | 121.97   |
| 20  | E8    | 207  | LEU  | C-N-CA | -6.56 | 110.16      | 121.97   |
| 6   | O8    | 178  | MET  | O-C-N  | -6.56 | 113.86      | 122.59   |
| 5   | P16   | 594  | ILE  | O-C-N  | -6.56 | 115.24      | 121.87   |
| 6   | O16   | 178  | MET  | O-C-N  | -6.56 | 113.86      | 122.59   |
| 21  | H     | 373  | MET  | O-C-N  | 6.56  | 129.63      | 122.15   |
| 5   | P     | 7    | GLU  | O-C-N  | -6.56 | 113.87      | 122.59   |
| 10  | C24   | 626  | GLN  | O-C-N  | -6.56 | 113.81      | 122.33   |
| 10  | C     | 881  | GLU  | O-C-N  | -6.56 | 114.96      | 123.02   |
| 21  | H8    | 138  | GLU  | O-C-N  | -6.56 | 113.96      | 122.61   |
| 18  | B     | 1962 | PRO  | CA-C-N | 6.55  | 132.80      | 122.51   |
| 18  | B     | 1962 | PRO  | C-N-CA | 6.55  | 132.80      | 122.51   |
| 11  | A16   | 467  | SER  | O-C-N  | -6.55 | 114.55      | 122.22   |
| 18  | B8    | 1768 | ILE  | CA-C-N | 6.55  | 131.67      | 122.36   |
| 18  | B8    | 1768 | ILE  | C-N-CA | 6.55  | 131.67      | 122.36   |
| 10  | C     | 1064 | PHE  | CA-C-N | 6.55  | 134.05      | 121.54   |
| 10  | C     | 1064 | PHE  | C-N-CA | 6.55  | 134.05      | 121.54   |
| 18  | B8    | 1289 | ASP  | CA-C-N | -6.55 | 112.13      | 121.50   |
| 18  | B8    | 1289 | ASP  | C-N-CA | -6.55 | 112.13      | 121.50   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 21  | H16   | 138  | GLU  | O-C-N  | -6.55 | 113.96      | 122.61   |
| 10  | C32   | 1771 | GLN  | O-C-N  | -6.55 | 113.42      | 122.46   |
| 7   | Q     | 6    | ASP  | CA-C-N | -6.55 | 111.73      | 122.54   |
| 7   | Q     | 6    | ASP  | C-N-CA | -6.55 | 111.73      | 122.54   |
| 12  | A48   | 467  | SER  | O-C-N  | -6.55 | 114.56      | 122.22   |
| 7   | Q8    | 6    | ASP  | CA-C-N | -6.55 | 111.74      | 122.54   |
| 7   | Q8    | 6    | ASP  | C-N-CA | -6.55 | 111.74      | 122.54   |
| 18  | B     | 1115 | VAL  | CA-C-N | 6.55  | 134.04      | 121.54   |
| 18  | B     | 1115 | VAL  | C-N-CA | 6.55  | 134.04      | 121.54   |
| 10  | C32   | 104  | GLU  | O-C-N  | -6.55 | 112.66      | 122.28   |
| 1   | R     | 1460 | MET  | CA-C-N | 6.54  | 129.43      | 120.46   |
| 1   | R     | 1460 | MET  | C-N-CA | 6.54  | 129.43      | 120.46   |
| 7   | Q16   | 6    | ASP  | CA-C-N | -6.54 | 111.74      | 122.54   |
| 7   | Q16   | 6    | ASP  | C-N-CA | -6.54 | 111.74      | 122.54   |
| 10  | C     | 1270 | SER  | CA-C-N | 6.54  | 130.71      | 121.02   |
| 10  | C     | 1270 | SER  | C-N-CA | 6.54  | 130.71      | 121.02   |
| 10  | C24   | 1543 | GLU  | CA-C-N | 6.54  | 134.23      | 121.41   |
| 10  | C24   | 1543 | GLU  | C-N-CA | 6.54  | 134.23      | 121.41   |
| 19  | 4     | 187  | SER  | O-C-N  | -6.54 | 113.89      | 122.59   |
| 22  | I8    | 270  | GLU  | O-C-N  | 6.54  | 128.81      | 122.07   |
| 10  | C32   | 1064 | PHE  | CA-C-N | 6.54  | 134.03      | 121.54   |
| 10  | C32   | 1064 | PHE  | C-N-CA | 6.54  | 134.03      | 121.54   |
| 10  | C24   | 1064 | PHE  | CA-C-N | 6.54  | 134.03      | 121.54   |
| 10  | C24   | 1064 | PHE  | C-N-CA | 6.54  | 134.03      | 121.54   |
| 18  | B8    | 614  | MET  | CA-C-N | 6.54  | 134.03      | 121.54   |
| 18  | B8    | 614  | MET  | C-N-CA | 6.54  | 134.03      | 121.54   |
| 10  | C32   | 626  | GLN  | O-C-N  | -6.54 | 113.83      | 122.33   |
| 18  | B     | 1768 | ILE  | CA-C-N | 6.54  | 131.64      | 122.36   |
| 18  | B     | 1768 | ILE  | C-N-CA | 6.54  | 131.64      | 122.36   |
| 21  | H     | 138  | GLU  | O-C-N  | -6.53 | 113.99      | 122.61   |
| 6   | O     | 178  | MET  | O-C-N  | -6.53 | 113.91      | 122.59   |
| 1   | R16   | 1460 | MET  | CA-C-N | 6.53  | 129.40      | 120.46   |
| 1   | R16   | 1460 | MET  | C-N-CA | 6.53  | 129.40      | 120.46   |
| 10  | C     | 404  | ASP  | O-C-N  | 6.53  | 129.04      | 122.12   |
| 18  | B     | 1289 | ASP  | CA-C-N | -6.53 | 112.17      | 121.50   |
| 18  | B     | 1289 | ASP  | C-N-CA | -6.53 | 112.17      | 121.50   |
| 1   | R8    | 1460 | MET  | CA-C-N | 6.52  | 129.40      | 120.46   |
| 1   | R8    | 1460 | MET  | C-N-CA | 6.52  | 129.40      | 120.46   |
| 8   | L8    | 149  | SER  | CA-C-N | 6.52  | 124.35      | 120.24   |
| 8   | L8    | 149  | SER  | C-N-CA | 6.52  | 124.35      | 120.24   |
| 18  | B8    | 1115 | VAL  | CA-C-N | 6.52  | 134.00      | 121.54   |
| 18  | B8    | 1115 | VAL  | C-N-CA | 6.52  | 134.00      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7   | Q16   | 352  | TRP  | CA-C-N | 6.52  | 132.26      | 122.68   |
| 7   | Q16   | 352  | TRP  | C-N-CA | 6.52  | 132.26      | 122.68   |
| 10  | C8    | 104  | GLU  | O-C-N  | -6.52 | 112.70      | 122.28   |
| 10  | C16   | 1064 | PHE  | CA-C-N | 6.51  | 133.98      | 121.54   |
| 10  | C16   | 1064 | PHE  | C-N-CA | 6.51  | 133.98      | 121.54   |
| 10  | C16   | 1771 | GLN  | O-C-N  | -6.51 | 113.47      | 122.46   |
| 10  | C8    | 1270 | SER  | CA-C-N | 6.51  | 130.66      | 121.02   |
| 10  | C8    | 1270 | SER  | C-N-CA | 6.51  | 130.66      | 121.02   |
| 5   | P     | 594  | ILE  | O-C-N  | -6.51 | 115.30      | 121.87   |
| 5   | P16   | 7    | GLU  | O-C-N  | -6.51 | 113.93      | 122.59   |
| 22  | I16   | 270  | GLU  | O-C-N  | 6.51  | 128.77      | 122.07   |
| 2   | M     | 335  | ALA  | CA-C-N | -6.50 | 110.91      | 120.28   |
| 2   | M     | 335  | ALA  | C-N-CA | -6.50 | 110.91      | 120.28   |
| 5   | P8    | 7    | GLU  | O-C-N  | -6.50 | 113.94      | 122.59   |
| 5   | P8    | 594  | ILE  | O-C-N  | -6.50 | 115.30      | 121.87   |
| 7   | Q     | 352  | TRP  | CA-C-N | 6.50  | 132.24      | 122.68   |
| 7   | Q     | 352  | TRP  | C-N-CA | 6.50  | 132.24      | 122.68   |
| 19  | 48    | 193  | LEU  | CA-C-N | -6.50 | 112.85      | 122.41   |
| 19  | 48    | 193  | LEU  | C-N-CA | -6.50 | 112.85      | 122.41   |
| 3   | N8    | 20   | ASP  | CA-C-N | 6.50  | 128.99      | 120.28   |
| 3   | N8    | 20   | ASP  | C-N-CA | 6.50  | 128.99      | 120.28   |
| 3   | N16   | 20   | ASP  | CA-C-N | 6.50  | 128.99      | 120.28   |
| 3   | N16   | 20   | ASP  | C-N-CA | 6.50  | 128.99      | 120.28   |
| 10  | C     | 1771 | GLN  | O-C-N  | -6.50 | 113.49      | 122.46   |
| 22  | I     | 270  | GLU  | O-C-N  | 6.50  | 128.76      | 122.07   |
| 10  | C24   | 1771 | GLN  | O-C-N  | -6.49 | 113.50      | 122.46   |
| 10  | C32   | 404  | ASP  | O-C-N  | 6.49  | 129.00      | 122.12   |
| 18  | B8    | 196  | ASP  | CA-C-N | 6.49  | 128.97      | 120.60   |
| 18  | B8    | 196  | ASP  | C-N-CA | 6.49  | 128.97      | 120.60   |
| 19  | 4     | 193  | LEU  | CA-C-N | -6.49 | 112.87      | 122.41   |
| 19  | 4     | 193  | LEU  | C-N-CA | -6.49 | 112.87      | 122.41   |
| 10  | C24   | 404  | ASP  | O-C-N  | 6.49  | 129.00      | 122.12   |
| 17  | F16   | 71   | GLU  | O-C-N  | -6.49 | 113.96      | 122.59   |
| 10  | C16   | 679  | ARG  | CA-C-N | 6.49  | 130.03      | 120.95   |
| 10  | C16   | 679  | ARG  | C-N-CA | 6.49  | 130.03      | 120.95   |
| 10  | C16   | 1543 | GLU  | CA-C-N | 6.49  | 134.12      | 121.41   |
| 10  | C16   | 1543 | GLU  | C-N-CA | 6.49  | 134.12      | 121.41   |
| 10  | C32   | 1270 | SER  | CA-C-N | 6.49  | 130.62      | 121.02   |
| 10  | C32   | 1270 | SER  | C-N-CA | 6.49  | 130.62      | 121.02   |
| 10  | C24   | 1270 | SER  | CA-C-N | 6.48  | 130.61      | 121.02   |
| 10  | C24   | 1270 | SER  | C-N-CA | 6.48  | 130.61      | 121.02   |
| 10  | C32   | 1543 | GLU  | CA-C-N | 6.48  | 134.12      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 1543 | GLU  | C-N-CA | 6.48  | 134.12      | 121.41   |
| 2   | M16   | 335  | ALA  | CA-C-N | -6.48 | 110.95      | 120.28   |
| 2   | M16   | 335  | ALA  | C-N-CA | -6.48 | 110.95      | 120.28   |
| 8   | L16   | 149  | SER  | CA-C-N | 6.48  | 124.32      | 120.24   |
| 8   | L16   | 149  | SER  | C-N-CA | 6.48  | 124.32      | 120.24   |
| 2   | M8    | 335  | ALA  | CA-C-N | -6.48 | 110.95      | 120.28   |
| 2   | M8    | 335  | ALA  | C-N-CA | -6.48 | 110.95      | 120.28   |
| 10  | C24   | 1223 | ASP  | CA-C-N | 6.48  | 131.32      | 122.19   |
| 10  | C24   | 1223 | ASP  | C-N-CA | 6.48  | 131.32      | 122.19   |
| 18  | B     | 1787 | LYS  | CA-C-N | 6.48  | 133.63      | 121.97   |
| 18  | B     | 1787 | LYS  | C-N-CA | 6.48  | 133.63      | 121.97   |
| 21  | H24   | 138  | GLU  | O-C-N  | -6.48 | 114.06      | 122.61   |
| 10  | C16   | 1270 | SER  | CA-C-N | 6.47  | 130.60      | 121.02   |
| 10  | C16   | 1270 | SER  | C-N-CA | 6.47  | 130.60      | 121.02   |
| 17  | F8    | 71   | GLU  | O-C-N  | -6.47 | 113.98      | 122.59   |
| 14  | W     | 608  | SER  | CA-C-N | -6.47 | 112.14      | 121.20   |
| 14  | W     | 608  | SER  | C-N-CA | -6.47 | 112.14      | 121.20   |
| 17  | F24   | 71   | GLU  | O-C-N  | -6.47 | 113.98      | 122.59   |
| 10  | C32   | 1066 | SER  | CA-C-N | 6.47  | 133.90      | 121.54   |
| 10  | C32   | 1066 | SER  | C-N-CA | 6.47  | 133.90      | 121.54   |
| 10  | C16   | 104  | GLU  | O-C-N  | -6.47 | 112.77      | 122.28   |
| 10  | C8    | 881  | GLU  | O-C-N  | -6.47 | 115.06      | 123.02   |
| 22  | I24   | 270  | GLU  | O-C-N  | 6.47  | 128.73      | 122.07   |
| 10  | C32   | 1600 | GLY  | O-C-N  | -6.46 | 115.49      | 122.73   |
| 7   | Q8    | 352  | TRP  | CA-C-N | 6.46  | 132.18      | 122.68   |
| 7   | Q8    | 352  | TRP  | C-N-CA | 6.46  | 132.18      | 122.68   |
| 10  | C24   | 679  | ARG  | CA-C-N | 6.46  | 129.99      | 120.95   |
| 10  | C24   | 679  | ARG  | C-N-CA | 6.46  | 129.99      | 120.95   |
| 10  | C24   | 104  | GLU  | O-C-N  | -6.46 | 112.79      | 122.28   |
| 10  | C8    | 1036 | SER  | CA-C-N | 6.46  | 130.00      | 120.90   |
| 10  | C8    | 1036 | SER  | C-N-CA | 6.46  | 130.00      | 120.90   |
| 18  | B     | 856  | LEU  | CA-C-N | 6.46  | 127.91      | 119.84   |
| 18  | B     | 856  | LEU  | C-N-CA | 6.46  | 127.91      | 119.84   |
| 18  | B8    | 1787 | LYS  | CA-C-N | 6.46  | 133.59      | 121.97   |
| 18  | B8    | 1787 | LYS  | C-N-CA | 6.46  | 133.59      | 121.97   |
| 10  | C     | 679  | ARG  | CA-C-N | 6.45  | 129.99      | 120.95   |
| 10  | C     | 679  | ARG  | C-N-CA | 6.45  | 129.99      | 120.95   |
| 18  | B     | 1288 | GLY  | CA-C-N | 6.45  | 133.87      | 121.54   |
| 18  | B     | 1288 | GLY  | C-N-CA | 6.45  | 133.87      | 121.54   |
| 10  | C32   | 679  | ARG  | CA-C-N | 6.45  | 129.99      | 120.95   |
| 10  | C32   | 679  | ARG  | C-N-CA | 6.45  | 129.99      | 120.95   |
| 18  | B     | 196  | ASP  | CA-C-N | 6.45  | 128.92      | 120.60   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 196  | ASP  | C-N-CA | 6.45  | 128.92      | 120.60   |
| 21  | H8    | 317  | ALA  | CA-C-N | -6.45 | 112.48      | 122.16   |
| 21  | H8    | 317  | ALA  | C-N-CA | -6.45 | 112.48      | 122.16   |
| 10  | C24   | 1445 | THR  | O-C-N  | -6.45 | 113.02      | 122.43   |
| 10  | C     | 1445 | THR  | O-C-N  | -6.45 | 113.02      | 122.43   |
| 10  | C     | 1036 | SER  | CA-C-N | 6.44  | 129.99      | 120.90   |
| 10  | C     | 1036 | SER  | C-N-CA | 6.44  | 129.99      | 120.90   |
| 18  | B     | 1288 | GLY  | O-C-N  | -6.44 | 114.33      | 122.70   |
| 18  | B     | 1792 | SER  | CA-C-N | 6.44  | 133.57      | 121.97   |
| 18  | B     | 1792 | SER  | C-N-CA | 6.44  | 133.57      | 121.97   |
| 10  | C16   | 1066 | SER  | CA-C-N | 6.44  | 133.84      | 121.54   |
| 10  | C16   | 1066 | SER  | C-N-CA | 6.44  | 133.84      | 121.54   |
| 20  | E     | 430  | ALA  | O-C-N  | -6.44 | 112.11      | 122.41   |
| 22  | I16   | 369  | HIS  | O-C-N  | -6.44 | 113.92      | 121.32   |
| 9   | K     | 1215 | GLY  | O-C-N  | -6.44 | 115.33      | 121.77   |
| 18  | B8    | 1792 | SER  | CA-C-N | 6.44  | 133.56      | 121.97   |
| 18  | B8    | 1792 | SER  | C-N-CA | 6.44  | 133.56      | 121.97   |
| 10  | C24   | 1066 | SER  | CA-C-N | 6.43  | 133.83      | 121.54   |
| 10  | C24   | 1066 | SER  | C-N-CA | 6.43  | 133.83      | 121.54   |
| 10  | C8    | 1066 | SER  | CA-C-N | 6.43  | 133.83      | 121.54   |
| 10  | C8    | 1066 | SER  | C-N-CA | 6.43  | 133.83      | 121.54   |
| 10  | C8    | 1445 | THR  | O-C-N  | -6.43 | 113.03      | 122.43   |
| 17  | F     | 71   | GLU  | O-C-N  | -6.43 | 114.04      | 122.59   |
| 18  | B8    | 972  | GLU  | O-C-N  | -6.43 | 113.88      | 122.43   |
| 2   | M     | 755  | THR  | O-C-N  | -6.43 | 115.21      | 122.93   |
| 9   | K8    | 1215 | GLY  | O-C-N  | -6.43 | 115.34      | 121.77   |
| 10  | C24   | 716  | THR  | O-C-N  | -6.43 | 114.04      | 122.59   |
| 10  | C16   | 1600 | GLY  | O-C-N  | -6.43 | 115.53      | 122.73   |
| 21  | H16   | 317  | ALA  | CA-C-N | -6.43 | 112.52      | 122.16   |
| 21  | H16   | 317  | ALA  | C-N-CA | -6.43 | 112.52      | 122.16   |
| 10  | C8    | 1543 | GLU  | CA-C-N | 6.42  | 134.00      | 121.41   |
| 10  | C8    | 1543 | GLU  | C-N-CA | 6.42  | 134.00      | 121.41   |
| 17  | F24   | 79   | ALA  | CA-C-N | 6.42  | 133.26      | 121.70   |
| 17  | F24   | 79   | ALA  | C-N-CA | 6.42  | 133.26      | 121.70   |
| 13  | V     | 816  | LYS  | O-C-N  | 6.42  | 129.47      | 122.15   |
| 18  | B     | 1311 | TRP  | CA-C-N | 6.42  | 128.89      | 120.28   |
| 18  | B     | 1311 | TRP  | C-N-CA | 6.42  | 128.89      | 120.28   |
| 10  | C16   | 1223 | ASP  | CA-C-N | 6.42  | 131.25      | 122.19   |
| 10  | C16   | 1223 | ASP  | C-N-CA | 6.42  | 131.25      | 122.19   |
| 20  | E8    | 430  | ALA  | O-C-N  | -6.42 | 112.14      | 122.41   |
| 10  | C16   | 1036 | SER  | CA-C-N | 6.42  | 129.95      | 120.90   |
| 10  | C16   | 1036 | SER  | C-N-CA | 6.42  | 129.95      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B8    | 509  | SER  | O-C-N      | -6.42 | 114.06      | 122.59   |
| 18  | B8    | 1127 | PRO  | O-C-N      | -6.42 | 113.89      | 121.46   |
| 18  | B8    | 1288 | GLY  | CA-C-N     | 6.42  | 133.80      | 121.54   |
| 18  | B8    | 1288 | GLY  | C-N-CA     | 6.42  | 133.80      | 121.54   |
| 10  | C8    | 679  | ARG  | CA-C-N     | 6.42  | 129.93      | 120.95   |
| 10  | C8    | 679  | ARG  | C-N-CA     | 6.42  | 129.93      | 120.95   |
| 18  | B8    | 1311 | TRP  | CA-C-N     | 6.42  | 128.88      | 120.28   |
| 18  | B8    | 1311 | TRP  | C-N-CA     | 6.42  | 128.88      | 120.28   |
| 18  | B     | 1127 | PRO  | O-C-N      | -6.42 | 113.89      | 121.46   |
| 10  | C     | 1066 | SER  | CA-C-N     | 6.41  | 133.79      | 121.54   |
| 10  | C     | 1066 | SER  | C-N-CA     | 6.41  | 133.79      | 121.54   |
| 10  | C24   | 1058 | GLU  | CA-C-N     | -6.41 | 112.19      | 120.65   |
| 10  | C24   | 1058 | GLU  | C-N-CA     | -6.41 | 112.19      | 120.65   |
| 18  | B8    | 316  | LEU  | O-C-N      | -6.41 | 114.49      | 122.82   |
| 18  | B8    | 1660 | SER  | O-C-N      | 6.41  | 129.72      | 122.22   |
| 2   | M16   | 755  | THR  | O-C-N      | -6.41 | 115.24      | 122.93   |
| 22  | I24   | 369  | HIS  | O-C-N      | -6.41 | 113.95      | 121.32   |
| 2   | M8    | 755  | THR  | O-C-N      | -6.41 | 115.24      | 122.93   |
| 10  | C16   | 1445 | THR  | O-C-N      | -6.41 | 113.08      | 122.43   |
| 10  | C32   | 1223 | ASP  | CA-C-N     | 6.41  | 131.22      | 122.19   |
| 10  | C32   | 1223 | ASP  | C-N-CA     | 6.41  | 131.22      | 122.19   |
| 10  | C     | 1600 | GLY  | O-C-N      | -6.40 | 115.56      | 122.73   |
| 17  | F16   | 79   | ALA  | CA-C-N     | 6.40  | 133.22      | 121.70   |
| 17  | F16   | 79   | ALA  | C-N-CA     | 6.40  | 133.22      | 121.70   |
| 18  | B     | 509  | SER  | O-C-N      | -6.40 | 114.08      | 122.59   |
| 24  | D40   | 277  | GLN  | OE1-CD-NE2 | -6.40 | 116.20      | 122.60   |
| 18  | B     | 316  | LEU  | O-C-N      | -6.40 | 114.50      | 122.82   |
| 2   | M     | 456  | ARG  | O-C-N      | 6.40  | 129.44      | 122.15   |
| 10  | C24   | 1052 | PHE  | CA-C-N     | 6.40  | 133.95      | 121.41   |
| 10  | C24   | 1052 | PHE  | C-N-CA     | 6.40  | 133.95      | 121.41   |
| 21  | H24   | 317  | ALA  | CA-C-N     | -6.40 | 112.56      | 122.16   |
| 21  | H24   | 317  | ALA  | C-N-CA     | -6.40 | 112.56      | 122.16   |
| 19  | 48    | 50   | THR  | CA-C-N     | -6.40 | 111.85      | 119.84   |
| 19  | 48    | 50   | THR  | C-N-CA     | -6.40 | 111.85      | 119.84   |
| 21  | H     | 317  | ALA  | CA-C-N     | -6.40 | 112.57      | 122.16   |
| 21  | H     | 317  | ALA  | C-N-CA     | -6.40 | 112.57      | 122.16   |
| 10  | C8    | 1600 | GLY  | O-C-N      | -6.39 | 115.57      | 122.73   |
| 18  | B8    | 1480 | HIS  | O-C-N      | -6.39 | 114.51      | 122.82   |
| 10  | C32   | 1445 | THR  | O-C-N      | -6.39 | 113.09      | 122.43   |
| 10  | C     | 1223 | ASP  | CA-C-N     | 6.39  | 131.21      | 122.19   |
| 10  | C     | 1223 | ASP  | C-N-CA     | 6.39  | 131.21      | 122.19   |
| 10  | C8    | 1223 | ASP  | CA-C-N     | 6.39  | 131.20      | 122.19   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10  | C8    | 1223 | ASP  | C-N-CA     | 6.39  | 131.20      | 122.19   |
| 18  | B     | 972  | GLU  | O-C-N      | -6.39 | 113.93      | 122.43   |
| 9   | K8    | 1221 | THR  | CA-C-N     | -6.39 | 110.11      | 121.81   |
| 9   | K8    | 1221 | THR  | C-N-CA     | -6.39 | 110.11      | 121.81   |
| 17  | F     | 79   | ALA  | CA-C-N     | 6.39  | 133.20      | 121.70   |
| 17  | F     | 79   | ALA  | C-N-CA     | 6.39  | 133.20      | 121.70   |
| 11  | A32   | 124  | ASN  | O-C-N      | -6.39 | 115.19      | 122.09   |
| 10  | C24   | 1036 | SER  | CA-C-N     | 6.39  | 129.91      | 120.90   |
| 10  | C24   | 1036 | SER  | C-N-CA     | 6.39  | 129.91      | 120.90   |
| 24  | D24   | 277  | GLN  | OE1-CD-NE2 | -6.39 | 116.21      | 122.60   |
| 9   | K     | 1177 | GLN  | O-C-N      | -6.38 | 113.65      | 122.46   |
| 19  | 48    | 196  | GLY  | O-C-N      | -6.38 | 114.40      | 122.70   |
| 10  | C32   | 530  | THR  | O-C-N      | -6.38 | 114.57      | 122.68   |
| 10  | C     | 1449 | GLU  | O-C-N      | 6.38  | 129.43      | 122.15   |
| 18  | B8    | 199  | LEU  | O-C-N      | 6.38  | 130.12      | 122.27   |
| 10  | C32   | 1036 | SER  | CA-C-N     | 6.38  | 129.89      | 120.90   |
| 10  | C32   | 1036 | SER  | C-N-CA     | 6.38  | 129.89      | 120.90   |
| 13  | V     | 869  | TYR  | O-C-N      | -6.38 | 114.04      | 122.33   |
| 22  | I     | 369  | HIS  | O-C-N      | -6.38 | 113.99      | 121.32   |
| 11  | A16   | 124  | ASN  | O-C-N      | -6.37 | 115.21      | 122.09   |
| 19  | 4     | 196  | GLY  | O-C-N      | -6.37 | 114.42      | 122.70   |
| 22  | I8    | 369  | HIS  | O-C-N      | -6.37 | 113.99      | 121.32   |
| 7   | Q16   | 218  | LYS  | O-C-N      | -6.37 | 115.18      | 123.02   |
| 10  | C16   | 1058 | GLU  | CA-C-N     | -6.37 | 112.24      | 120.65   |
| 10  | C16   | 1058 | GLU  | C-N-CA     | -6.37 | 112.24      | 120.65   |
| 10  | C8    | 1052 | PHE  | CA-C-N     | 6.37  | 133.90      | 121.41   |
| 10  | C8    | 1052 | PHE  | C-N-CA     | 6.37  | 133.90      | 121.41   |
| 10  | C32   | 1052 | PHE  | CA-C-N     | 6.37  | 133.90      | 121.41   |
| 10  | C32   | 1052 | PHE  | C-N-CA     | 6.37  | 133.90      | 121.41   |
| 10  | C32   | 716  | THR  | O-C-N      | -6.37 | 114.12      | 122.59   |
| 10  | C32   | 1058 | GLU  | CA-C-N     | -6.37 | 112.25      | 120.65   |
| 10  | C32   | 1058 | GLU  | C-N-CA     | -6.37 | 112.25      | 120.65   |
| 10  | C24   | 1600 | GLY  | O-C-N      | -6.36 | 115.60      | 122.73   |
| 24  | D8    | 277  | GLN  | OE1-CD-NE2 | -6.36 | 116.24      | 122.60   |
| 2   | M8    | 456  | ARG  | O-C-N      | 6.36  | 129.40      | 122.15   |
| 18  | B     | 199  | LEU  | O-C-N      | 6.36  | 130.09      | 122.27   |
| 18  | B     | 1480 | HIS  | O-C-N      | -6.36 | 114.55      | 122.82   |
| 10  | C16   | 1052 | PHE  | CA-C-N     | 6.36  | 133.87      | 121.41   |
| 10  | C16   | 1052 | PHE  | C-N-CA     | 6.36  | 133.87      | 121.41   |
| 18  | B8    | 1714 | MET  | CA-C-N     | 6.36  | 128.80      | 120.28   |
| 18  | B8    | 1714 | MET  | C-N-CA     | 6.36  | 128.80      | 120.28   |
| 9   | K8    | 1177 | GLN  | O-C-N      | -6.35 | 113.69      | 122.46   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 716  | THR  | O-C-N  | -6.35 | 114.14      | 122.59   |
| 12  | A     | 335  | ASP  | CA-C-N | 6.35  | 130.76      | 120.60   |
| 12  | A     | 335  | ASP  | C-N-CA | 6.35  | 130.76      | 120.60   |
| 2   | M     | 202  | LYS  | CA-C-N | -6.35 | 113.42      | 119.90   |
| 2   | M     | 202  | LYS  | C-N-CA | -6.35 | 113.42      | 119.90   |
| 7   | Q16   | 295  | SER  | O-C-N  | -6.35 | 115.50      | 123.05   |
| 20  | E8    | 493  | TRP  | O-C-N  | -6.35 | 114.90      | 122.27   |
| 9   | K     | 1221 | THR  | CA-C-N | -6.35 | 110.19      | 121.81   |
| 9   | K     | 1221 | THR  | C-N-CA | -6.35 | 110.19      | 121.81   |
| 10  | C16   | 530  | THR  | O-C-N  | -6.35 | 114.62      | 122.68   |
| 19  | 4     | 50   | THR  | CA-C-N | -6.35 | 111.91      | 119.84   |
| 19  | 4     | 50   | THR  | C-N-CA | -6.35 | 111.91      | 119.84   |
| 17  | F8    | 79   | ALA  | CA-C-N | 6.35  | 133.12      | 121.70   |
| 17  | F8    | 79   | ALA  | C-N-CA | 6.35  | 133.12      | 121.70   |
| 2   | M     | 625  | HIS  | O-C-N  | 6.34  | 126.37      | 121.23   |
| 7   | Q     | 218  | LYS  | O-C-N  | -6.34 | 115.22      | 123.02   |
| 11  | A24   | 335  | ASP  | CA-C-N | 6.34  | 130.75      | 120.60   |
| 11  | A24   | 335  | ASP  | C-N-CA | 6.34  | 130.75      | 120.60   |
| 13  | V     | 805  | LEU  | O-C-N  | 6.34  | 129.38      | 122.15   |
| 20  | E     | 493  | TRP  | O-C-N  | -6.34 | 114.92      | 122.27   |
| 23  | J16   | 726  | GLY  | CA-C-N | -6.34 | 112.95      | 119.98   |
| 23  | J16   | 726  | GLY  | C-N-CA | -6.34 | 112.95      | 119.98   |
| 10  | C16   | 1666 | LYS  | O-C-N  | -6.33 | 115.81      | 123.29   |
| 18  | B     | 671  | MET  | O-C-N  | -6.33 | 114.58      | 122.82   |
| 7   | Q16   | 222  | PHE  | CA-C-N | 6.33  | 133.64      | 121.54   |
| 7   | Q16   | 222  | PHE  | C-N-CA | 6.33  | 133.64      | 121.54   |
| 10  | C     | 716  | THR  | O-C-N  | -6.33 | 114.17      | 122.59   |
| 12  | A48   | 335  | ASP  | CA-C-N | 6.33  | 130.73      | 120.60   |
| 12  | A48   | 335  | ASP  | C-N-CA | 6.33  | 130.73      | 120.60   |
| 2   | M16   | 456  | ARG  | O-C-N  | 6.33  | 129.37      | 122.15   |
| 7   | Q8    | 218  | LYS  | O-C-N  | -6.33 | 115.23      | 123.02   |
| 10  | C8    | 1058 | GLU  | CA-C-N | -6.33 | 112.29      | 120.65   |
| 10  | C8    | 1058 | GLU  | C-N-CA | -6.33 | 112.29      | 120.65   |
| 2   | M16   | 202  | LYS  | CA-C-N | -6.33 | 113.44      | 119.90   |
| 2   | M16   | 202  | LYS  | C-N-CA | -6.33 | 113.44      | 119.90   |
| 7   | Q8    | 222  | PHE  | CA-C-N | 6.33  | 133.63      | 121.54   |
| 7   | Q8    | 222  | PHE  | C-N-CA | 6.33  | 133.63      | 121.54   |
| 3   | N16   | 181  | SER  | CA-C-N | 6.33  | 126.55      | 122.18   |
| 3   | N16   | 181  | SER  | C-N-CA | 6.33  | 126.55      | 122.18   |
| 10  | C     | 1052 | PHE  | CA-C-N | 6.33  | 133.81      | 121.41   |
| 10  | C     | 1052 | PHE  | C-N-CA | 6.33  | 133.81      | 121.41   |
| 8   | L8    | 973  | THR  | CA-C-N | 6.33  | 133.09      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | L8    | 973  | THR  | C-N-CA     | 6.33  | 133.09      | 121.70   |
| 10  | C8    | 1161 | PHE  | CA-C-N     | -6.33 | 111.93      | 119.84   |
| 10  | C8    | 1161 | PHE  | C-N-CA     | -6.33 | 111.93      | 119.84   |
| 10  | C32   | 1795 | ASP  | CA-C-N     | 6.33  | 128.66      | 120.44   |
| 10  | C32   | 1795 | ASP  | C-N-CA     | 6.33  | 128.66      | 120.44   |
| 11  | A16   | 335  | ASP  | CA-C-N     | 6.32  | 130.71      | 120.60   |
| 11  | A16   | 335  | ASP  | C-N-CA     | 6.32  | 130.71      | 120.60   |
| 18  | B8    | 1288 | GLY  | O-C-N      | -6.32 | 114.49      | 122.70   |
| 10  | C8    | 1449 | GLU  | O-C-N      | 6.32  | 129.35      | 122.15   |
| 10  | C     | 1058 | GLU  | CA-C-N     | -6.32 | 112.31      | 120.65   |
| 10  | C     | 1058 | GLU  | C-N-CA     | -6.32 | 112.31      | 120.65   |
| 18  | B     | 1660 | SER  | O-C-N      | 6.32  | 129.61      | 122.22   |
| 18  | B     | 1961 | TYR  | CA-C-N     | -6.32 | 113.01      | 119.83   |
| 18  | B     | 1961 | TYR  | C-N-CA     | -6.32 | 113.01      | 119.83   |
| 7   | Q     | 222  | PHE  | CA-C-N     | 6.31  | 133.60      | 121.54   |
| 7   | Q     | 222  | PHE  | C-N-CA     | 6.31  | 133.60      | 121.54   |
| 10  | C32   | 1721 | GLN  | O-C-N      | 6.31  | 130.89      | 122.43   |
| 7   | Q8    | 295  | SER  | O-C-N      | -6.31 | 115.54      | 123.05   |
| 18  | B     | 1714 | MET  | CA-C-N     | 6.31  | 128.73      | 120.28   |
| 18  | B     | 1714 | MET  | C-N-CA     | 6.31  | 128.73      | 120.28   |
| 18  | B8    | 1787 | LYS  | O-C-N      | -6.31 | 114.20      | 122.59   |
| 10  | C24   | 1666 | LYS  | O-C-N      | -6.30 | 115.85      | 123.29   |
| 8   | L16   | 973  | THR  | CA-C-N     | 6.30  | 133.04      | 121.70   |
| 8   | L16   | 973  | THR  | C-N-CA     | 6.30  | 133.04      | 121.70   |
| 10  | C16   | 1449 | GLU  | O-C-N      | 6.30  | 129.33      | 122.15   |
| 10  | C24   | 1721 | GLN  | O-C-N      | 6.30  | 130.87      | 122.43   |
| 23  | J8    | 726  | GLY  | CA-C-N     | -6.30 | 112.99      | 119.98   |
| 23  | J8    | 726  | GLY  | C-N-CA     | -6.30 | 112.99      | 119.98   |
| 24  | D     | 277  | GLN  | OE1-CD-NE2 | -6.30 | 116.30      | 122.60   |
| 24  | D16   | 277  | GLN  | OE1-CD-NE2 | -6.30 | 116.30      | 122.60   |
| 3   | N     | 181  | SER  | CA-C-N     | 6.29  | 126.52      | 122.18   |
| 3   | N     | 181  | SER  | C-N-CA     | 6.29  | 126.52      | 122.18   |
| 14  | W     | 593  | GLY  | O-C-N      | -6.29 | 115.47      | 121.77   |
| 7   | Q     | 295  | SER  | O-C-N      | -6.29 | 115.56      | 123.05   |
| 18  | B     | 1787 | LYS  | O-C-N      | -6.29 | 114.22      | 122.59   |
| 18  | B8    | 671  | MET  | O-C-N      | -6.29 | 114.64      | 122.82   |
| 18  | B8    | 1785 | LYS  | O-C-N      | -6.29 | 114.09      | 121.32   |
| 9   | K     | 1233 | ARG  | O-C-N      | -6.29 | 115.06      | 123.23   |
| 10  | C24   | 1546 | ASN  | CA-C-N     | 6.29  | 129.56      | 120.38   |
| 10  | C24   | 1546 | ASN  | C-N-CA     | 6.29  | 129.56      | 120.38   |
| 18  | B8    | 1961 | TYR  | CA-C-N     | -6.29 | 113.04      | 119.83   |
| 18  | B8    | 1961 | TYR  | C-N-CA     | -6.29 | 113.04      | 119.83   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | N8    | 181  | SER  | CA-C-N     | 6.28  | 126.52      | 122.18   |
| 3   | N8    | 181  | SER  | C-N-CA     | 6.28  | 126.52      | 122.18   |
| 10  | C16   | 1499 | ASN  | O-C-N      | -6.28 | 114.23      | 122.59   |
| 10  | C16   | 1546 | ASN  | CA-C-N     | 6.28  | 129.55      | 120.38   |
| 10  | C16   | 1546 | ASN  | C-N-CA     | 6.28  | 129.55      | 120.38   |
| 10  | C24   | 1795 | ASP  | CA-C-N     | 6.28  | 128.60      | 120.44   |
| 10  | C24   | 1795 | ASP  | C-N-CA     | 6.28  | 128.60      | 120.44   |
| 19  | 48    | 56   | GLU  | CA-C-N     | -6.28 | 109.55      | 121.54   |
| 19  | 48    | 56   | GLU  | C-N-CA     | -6.28 | 109.55      | 121.54   |
| 24  | D32   | 277  | GLN  | OE1-CD-NE2 | -6.28 | 116.32      | 122.60   |
| 10  | C32   | 522  | GLU  | O-C-N      | 6.28  | 129.31      | 122.15   |
| 9   | K8    | 1233 | ARG  | O-C-N      | -6.28 | 115.07      | 123.23   |
| 10  | C8    | 522  | GLU  | O-C-N      | 6.28  | 129.30      | 122.15   |
| 10  | C32   | 1161 | PHE  | CA-C-N     | -6.28 | 112.00      | 119.84   |
| 10  | C32   | 1161 | PHE  | C-N-CA     | -6.28 | 112.00      | 119.84   |
| 10  | C32   | 1666 | LYS  | O-C-N      | -6.28 | 115.88      | 123.29   |
| 10  | C8    | 1795 | ASP  | CA-C-N     | 6.27  | 128.60      | 120.44   |
| 10  | C8    | 1795 | ASP  | C-N-CA     | 6.27  | 128.60      | 120.44   |
| 23  | J32   | 726  | GLY  | CA-C-N     | -6.27 | 113.02      | 119.98   |
| 23  | J32   | 726  | GLY  | C-N-CA     | -6.27 | 113.02      | 119.98   |
| 8   | L     | 973  | THR  | CA-C-N     | 6.27  | 132.99      | 121.70   |
| 8   | L     | 973  | THR  | C-N-CA     | 6.27  | 132.99      | 121.70   |
| 10  | C16   | 1285 | VAL  | O-C-N      | 6.27  | 128.89      | 121.80   |
| 10  | C8    | 1721 | GLN  | O-C-N      | 6.27  | 130.83      | 122.43   |
| 2   | M8    | 202  | LYS  | CA-C-N     | -6.27 | 113.50      | 119.90   |
| 2   | M8    | 202  | LYS  | C-N-CA     | -6.27 | 113.50      | 119.90   |
| 10  | C     | 1161 | PHE  | CA-C-N     | -6.27 | 112.00      | 119.84   |
| 10  | C     | 1161 | PHE  | C-N-CA     | -6.27 | 112.00      | 119.84   |
| 11  | A32   | 335  | ASP  | CA-C-N     | 6.27  | 130.63      | 120.60   |
| 11  | A32   | 335  | ASP  | C-N-CA     | 6.27  | 130.63      | 120.60   |
| 19  | 48    | 99   | GLU  | CA-C-N     | -6.27 | 110.69      | 121.97   |
| 19  | 48    | 99   | GLU  | C-N-CA     | -6.27 | 110.69      | 121.97   |
| 10  | C16   | 1795 | ASP  | CA-C-N     | 6.27  | 128.59      | 120.44   |
| 10  | C16   | 1795 | ASP  | C-N-CA     | 6.27  | 128.59      | 120.44   |
| 11  | A40   | 335  | ASP  | CA-C-N     | 6.26  | 130.62      | 120.60   |
| 11  | A40   | 335  | ASP  | C-N-CA     | 6.26  | 130.62      | 120.60   |
| 10  | C24   | 1075 | ASP  | O-C-N      | -6.26 | 114.26      | 122.59   |
| 10  | C16   | 1161 | PHE  | CA-C-N     | -6.26 | 112.01      | 119.84   |
| 10  | C16   | 1161 | PHE  | C-N-CA     | -6.26 | 112.01      | 119.84   |
| 18  | B     | 1785 | LYS  | O-C-N      | -6.26 | 114.12      | 121.32   |
| 19  | 4     | 56   | GLU  | CA-C-N     | -6.26 | 109.58      | 121.54   |
| 19  | 4     | 56   | GLU  | C-N-CA     | -6.26 | 109.58      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K8    | 892  | GLU  | CA-C-N | -6.26 | 112.59      | 122.23   |
| 9   | K8    | 892  | GLU  | C-N-CA | -6.26 | 112.59      | 122.23   |
| 10  | C24   | 1161 | PHE  | CA-C-N | -6.26 | 112.01      | 119.84   |
| 10  | C24   | 1161 | PHE  | C-N-CA | -6.26 | 112.01      | 119.84   |
| 10  | C     | 1666 | LYS  | O-C-N  | -6.26 | 115.90      | 123.29   |
| 10  | C16   | 1721 | GLN  | O-C-N  | 6.26  | 130.81      | 122.43   |
| 10  | C32   | 1285 | VAL  | O-C-N  | 6.26  | 128.87      | 121.80   |
| 10  | C8    | 1250 | ALA  | O-C-N  | 6.26  | 128.75      | 122.12   |
| 9   | K     | 892  | GLU  | CA-C-N | -6.25 | 112.60      | 122.23   |
| 9   | K     | 892  | GLU  | C-N-CA | -6.25 | 112.60      | 122.23   |
| 10  | C     | 1285 | VAL  | O-C-N  | 6.25  | 128.87      | 121.80   |
| 10  | C24   | 1285 | VAL  | O-C-N  | 6.25  | 128.87      | 121.80   |
| 10  | C32   | 1499 | ASN  | O-C-N  | -6.25 | 114.27      | 122.59   |
| 10  | C     | 1721 | GLN  | O-C-N  | 6.25  | 130.81      | 122.43   |
| 19  | 4     | 99   | GLU  | CA-C-N | -6.25 | 110.72      | 121.97   |
| 19  | 4     | 99   | GLU  | C-N-CA | -6.25 | 110.72      | 121.97   |
| 10  | C     | 669  | GLY  | CA-C-N | 6.25  | 129.79      | 123.04   |
| 10  | C     | 669  | GLY  | C-N-CA | 6.25  | 129.79      | 123.04   |
| 18  | B8    | 347  | SER  | CA-C-N | 6.25  | 126.72      | 119.47   |
| 18  | B8    | 347  | SER  | C-N-CA | 6.25  | 126.72      | 119.47   |
| 18  | B     | 347  | SER  | CA-C-N | 6.25  | 126.72      | 119.47   |
| 18  | B     | 347  | SER  | C-N-CA | 6.25  | 126.72      | 119.47   |
| 18  | B     | 7    | VAL  | CA-C-N | 6.24  | 129.62      | 120.82   |
| 18  | B     | 7    | VAL  | C-N-CA | 6.24  | 129.62      | 120.82   |
| 18  | B8    | 7    | VAL  | CA-C-N | 6.24  | 129.62      | 120.82   |
| 18  | B8    | 7    | VAL  | C-N-CA | 6.24  | 129.62      | 120.82   |
| 10  | C     | 522  | GLU  | O-C-N  | 6.24  | 129.26      | 122.15   |
| 2   | M8    | 625  | HIS  | O-C-N  | 6.24  | 126.28      | 121.23   |
| 10  | C32   | 1546 | ASN  | CA-C-N | 6.24  | 129.48      | 120.38   |
| 10  | C32   | 1546 | ASN  | C-N-CA | 6.24  | 129.48      | 120.38   |
| 23  | J24   | 726  | GLY  | CA-C-N | -6.23 | 113.06      | 119.98   |
| 23  | J24   | 726  | GLY  | C-N-CA | -6.23 | 113.06      | 119.98   |
| 2   | M16   | 625  | HIS  | O-C-N  | 6.23  | 126.28      | 121.23   |
| 10  | C16   | 1452 | GLN  | O-C-N  | 6.23  | 128.72      | 122.12   |
| 10  | C24   | 1449 | GLU  | O-C-N  | 6.23  | 129.25      | 122.15   |
| 10  | C     | 1691 | GLU  | O-C-N  | 6.23  | 128.81      | 122.09   |
| 20  | E     | 418  | THR  | O-C-N  | -6.23 | 113.82      | 122.41   |
| 20  | E8    | 201  | LEU  | O-C-N  | -6.23 | 114.77      | 122.68   |
| 10  | C32   | 1452 | GLN  | O-C-N  | 6.22  | 128.72      | 122.12   |
| 10  | C     | 1795 | ASP  | CA-C-N | 6.22  | 128.53      | 120.44   |
| 10  | C     | 1795 | ASP  | C-N-CA | 6.22  | 128.53      | 120.44   |
| 10  | C16   | 1075 | ASP  | O-C-N  | -6.22 | 114.32      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 1499 | ASN  | O-C-N  | -6.22 | 114.32      | 122.59   |
| 20  | E8    | 418  | THR  | O-C-N  | -6.22 | 113.83      | 122.41   |
| 10  | C8    | 1691 | GLU  | O-C-N  | 6.22  | 128.80      | 122.09   |
| 10  | C16   | 1277 | SER  | O-C-N  | -6.21 | 115.66      | 123.05   |
| 10  | C8    | 1452 | GLN  | O-C-N  | 6.21  | 128.71      | 122.12   |
| 10  | C     | 1499 | ASN  | O-C-N  | -6.21 | 114.33      | 122.59   |
| 3   | N     | 220  | PRO  | O-C-N  | -6.21 | 116.45      | 123.03   |
| 10  | C16   | 522  | GLU  | O-C-N  | 6.21  | 129.23      | 122.15   |
| 15  | J     | 644  | ARG  | O-C-N  | 6.21  | 128.70      | 122.12   |
| 10  | C32   | 1449 | GLU  | O-C-N  | 6.20  | 129.22      | 122.15   |
| 1   | R16   | 1146 | ASP  | CA-C-N | 6.20  | 133.39      | 121.54   |
| 1   | R16   | 1146 | ASP  | C-N-CA | 6.20  | 133.39      | 121.54   |
| 10  | C     | 1546 | ASN  | CA-C-N | 6.20  | 129.43      | 120.38   |
| 10  | C     | 1546 | ASN  | C-N-CA | 6.20  | 129.43      | 120.38   |
| 10  | C16   | 1661 | LEU  | CA-C-N | -6.20 | 109.70      | 121.54   |
| 10  | C16   | 1661 | LEU  | C-N-CA | -6.20 | 109.70      | 121.54   |
| 10  | C32   | 1661 | LEU  | CA-C-N | -6.20 | 109.70      | 121.54   |
| 10  | C32   | 1661 | LEU  | C-N-CA | -6.20 | 109.70      | 121.54   |
| 10  | C     | 1452 | GLN  | O-C-N  | 6.19  | 128.69      | 122.12   |
| 10  | C8    | 1499 | ASN  | O-C-N  | -6.19 | 114.35      | 122.59   |
| 1   | R8    | 1146 | ASP  | CA-C-N | 6.19  | 133.37      | 121.54   |
| 1   | R8    | 1146 | ASP  | C-N-CA | 6.19  | 133.37      | 121.54   |
| 10  | C24   | 669  | GLY  | CA-C-N | 6.19  | 129.73      | 123.04   |
| 10  | C24   | 669  | GLY  | C-N-CA | 6.19  | 129.73      | 123.04   |
| 10  | C8    | 1285 | VAL  | O-C-N  | 6.19  | 128.79      | 121.80   |
| 18  | B8    | 994  | CYS  | O-C-N  | -6.19 | 114.36      | 122.59   |
| 10  | C32   | 669  | GLY  | CA-C-N | 6.19  | 129.73      | 123.04   |
| 10  | C32   | 669  | GLY  | C-N-CA | 6.19  | 129.73      | 123.04   |
| 10  | C     | 1250 | ALA  | O-C-N  | 6.19  | 128.68      | 122.12   |
| 10  | C24   | 1668 | ARG  | O-C-N  | -6.19 | 114.36      | 122.59   |
| 1   | R     | 1146 | ASP  | CA-C-N | 6.18  | 133.35      | 121.54   |
| 1   | R     | 1146 | ASP  | C-N-CA | 6.18  | 133.35      | 121.54   |
| 19  | 48    | 191  | GLY  | O-C-N  | 6.18  | 129.55      | 122.38   |
| 24  | D24   | 761  | ASN  | N-CA-C | 6.18  | 123.97      | 110.80   |
| 10  | C24   | 1250 | ALA  | O-C-N  | 6.18  | 128.67      | 122.12   |
| 12  | A     | 794  | THR  | O-C-N  | -6.18 | 115.33      | 122.93   |
| 10  | C     | 1075 | ASP  | O-C-N  | -6.18 | 114.37      | 122.59   |
| 9   | K     | 604  | SER  | O-C-N  | -6.18 | 114.67      | 122.27   |
| 10  | C     | 621  | VAL  | O-C-N  | -6.18 | 115.72      | 122.64   |
| 10  | C24   | 455  | GLY  | CA-C-N | -6.18 | 114.00      | 123.14   |
| 10  | C24   | 455  | GLY  | C-N-CA | -6.18 | 114.00      | 123.14   |
| 10  | C     | 1661 | LEU  | CA-C-N | -6.18 | 109.74      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C     | 1661 | LEU  | C-N-CA | -6.18 | 109.74      | 121.54   |
| 19  | 48    | 65   | LYS  | O-C-N  | -6.18 | 114.38      | 122.59   |
| 10  | C32   | 1668 | ARG  | O-C-N  | -6.18 | 114.38      | 122.59   |
| 13  | V     | 814  | MET  | O-C-N  | 6.17  | 128.43      | 122.07   |
| 10  | C     | 1668 | ARG  | O-C-N  | -6.17 | 114.38      | 122.59   |
| 21  | H16   | 292  | LYS  | O-C-N  | -6.17 | 116.09      | 123.31   |
| 24  | D32   | 761  | ASN  | N-CA-C | 6.17  | 123.95      | 110.80   |
| 10  | C24   | 1661 | LEU  | CA-C-N | -6.17 | 109.75      | 121.54   |
| 10  | C24   | 1661 | LEU  | C-N-CA | -6.17 | 109.75      | 121.54   |
| 10  | C8    | 1075 | ASP  | O-C-N  | -6.17 | 114.38      | 122.59   |
| 24  | D     | 761  | ASN  | N-CA-C | 6.17  | 123.95      | 110.80   |
| 18  | B8    | 1119 | LYS  | O-C-N  | -6.17 | 115.00      | 122.22   |
| 20  | E     | 201  | LEU  | O-C-N  | -6.17 | 114.84      | 122.68   |
| 10  | C     | 426  | LEU  | O-C-N  | -6.17 | 115.12      | 122.15   |
| 23  | J24   | 731  | LEU  | CA-C-N | -6.17 | 111.96      | 122.56   |
| 23  | J24   | 731  | LEU  | C-N-CA | -6.17 | 111.96      | 122.56   |
| 10  | C32   | 1075 | ASP  | O-C-N  | -6.17 | 114.39      | 122.59   |
| 10  | C8    | 669  | GLY  | CA-C-N | 6.16  | 129.70      | 123.04   |
| 10  | C8    | 669  | GLY  | C-N-CA | 6.16  | 129.70      | 123.04   |
| 18  | B     | 1119 | LYS  | O-C-N  | -6.16 | 115.01      | 122.22   |
| 18  | B     | 1730 | ALA  | O-C-N  | 6.16  | 128.65      | 122.12   |
| 24  | D40   | 761  | ASN  | N-CA-C | 6.16  | 123.93      | 110.80   |
| 19  | 4     | 65   | LYS  | O-C-N  | -6.16 | 114.39      | 122.59   |
| 21  | H     | 292  | LYS  | O-C-N  | -6.16 | 116.10      | 123.31   |
| 24  | D8    | 761  | ASN  | N-CA-C | 6.16  | 123.92      | 110.80   |
| 9   | K     | 1069 | PRO  | O-C-N  | -6.16 | 114.32      | 122.64   |
| 9   | K8    | 1069 | PRO  | O-C-N  | -6.16 | 114.32      | 122.64   |
| 10  | C     | 455  | GLY  | CA-C-N | -6.16 | 114.02      | 123.14   |
| 10  | C     | 455  | GLY  | C-N-CA | -6.16 | 114.02      | 123.14   |
| 10  | C24   | 621  | VAL  | O-C-N  | -6.16 | 115.74      | 122.64   |
| 18  | B     | 4    | PRO  | O-C-N  | -6.16 | 114.33      | 122.64   |
| 18  | B8    | 1133 | THR  | CA-C-N | 6.16  | 133.30      | 121.54   |
| 18  | B8    | 1133 | THR  | C-N-CA | 6.16  | 133.30      | 121.54   |
| 24  | D16   | 761  | ASN  | N-CA-C | 6.16  | 123.91      | 110.80   |
| 10  | C8    | 1357 | LEU  | O-C-N  | -6.16 | 114.40      | 122.59   |
| 10  | C8    | 1546 | ASN  | CA-C-N | 6.16  | 129.37      | 120.38   |
| 10  | C8    | 1546 | ASN  | C-N-CA | 6.16  | 129.37      | 120.38   |
| 2   | M16   | 448  | ASP  | O-C-N  | -6.15 | 114.41      | 122.59   |
| 9   | K8    | 604  | SER  | O-C-N  | -6.15 | 114.70      | 122.27   |
| 2   | M8    | 448  | ASP  | O-C-N  | -6.15 | 114.41      | 122.59   |
| 7   | Q     | 277  | ASN  | O-C-N  | 6.15  | 128.39      | 121.32   |
| 18  | B     | 1133 | THR  | CA-C-N | 6.15  | 133.29      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 1133 | THR  | C-N-CA | 6.15  | 133.29      | 121.54   |
| 18  | B     | 1793 | ILE  | O-C-N  | -6.15 | 114.88      | 122.57   |
| 10  | C32   | 621  | VAL  | O-C-N  | -6.15 | 115.75      | 122.64   |
| 3   | N16   | 220  | PRO  | O-C-N  | -6.15 | 116.52      | 123.03   |
| 10  | C24   | 1357 | LEU  | O-C-N  | -6.15 | 114.42      | 122.59   |
| 21  | H24   | 292  | LYS  | O-C-N  | -6.14 | 116.12      | 123.31   |
| 10  | C16   | 1443 | ASP  | CA-C-N | 6.14  | 133.45      | 121.41   |
| 10  | C16   | 1443 | ASP  | C-N-CA | 6.14  | 133.45      | 121.41   |
| 10  | C32   | 426  | LEU  | O-C-N  | -6.14 | 115.15      | 122.15   |
| 10  | C32   | 594  | LYS  | O-C-N  | 6.14  | 128.63      | 122.12   |
| 11  | A24   | 794  | THR  | O-C-N  | -6.14 | 115.38      | 122.93   |
| 10  | C8    | 426  | LEU  | O-C-N  | -6.14 | 115.15      | 122.15   |
| 10  | C32   | 1544 | GLY  | CA-C-N | -6.14 | 112.72      | 122.29   |
| 10  | C32   | 1544 | GLY  | C-N-CA | -6.14 | 112.72      | 122.29   |
| 23  | J32   | 731  | LEU  | CA-C-N | -6.13 | 112.01      | 122.56   |
| 23  | J32   | 731  | LEU  | C-N-CA | -6.13 | 112.01      | 122.56   |
| 10  | C32   | 1357 | LEU  | O-C-N  | -6.13 | 114.43      | 122.59   |
| 10  | C24   | 522  | GLU  | O-C-N  | 6.13  | 129.14      | 122.15   |
| 10  | C32   | 455  | GLY  | CA-C-N | -6.13 | 114.06      | 123.14   |
| 10  | C32   | 455  | GLY  | C-N-CA | -6.13 | 114.06      | 123.14   |
| 5   | P16   | 18   | THR  | CA-C-N | -6.13 | 112.83      | 121.72   |
| 5   | P16   | 18   | THR  | C-N-CA | -6.13 | 112.83      | 121.72   |
| 10  | C16   | 1691 | GLU  | O-C-N  | 6.13  | 128.71      | 122.09   |
| 18  | B8    | 1730 | ALA  | O-C-N  | 6.13  | 128.62      | 122.12   |
| 19  | 4     | 191  | GLY  | O-C-N  | 6.13  | 129.49      | 122.38   |
| 10  | C32   | 1250 | ALA  | O-C-N  | 6.13  | 128.62      | 122.12   |
| 10  | C16   | 621  | VAL  | O-C-N  | -6.13 | 115.78      | 122.64   |
| 18  | B     | 994  | CYS  | O-C-N  | -6.13 | 114.44      | 122.59   |
| 23  | J8    | 731  | LEU  | CA-C-N | -6.13 | 112.02      | 122.56   |
| 23  | J8    | 731  | LEU  | C-N-CA | -6.13 | 112.02      | 122.56   |
| 7   | Q     | 92   | GLY  | CA-C-N | 6.13  | 133.42      | 121.41   |
| 7   | Q     | 92   | GLY  | C-N-CA | 6.13  | 133.42      | 121.41   |
| 5   | P     | 142  | SER  | O-C-N  | -6.13 | 115.87      | 123.04   |
| 10  | C16   | 669  | GLY  | CA-C-N | 6.13  | 129.66      | 123.04   |
| 10  | C16   | 669  | GLY  | C-N-CA | 6.13  | 129.66      | 123.04   |
| 18  | B8    | 1793 | ILE  | O-C-N  | -6.13 | 114.91      | 122.57   |
| 5   | P8    | 142  | SER  | O-C-N  | -6.12 | 115.88      | 123.04   |
| 10  | C16   | 1668 | ARG  | O-C-N  | -6.12 | 114.44      | 122.59   |
| 18  | B8    | 4    | PRO  | O-C-N  | -6.12 | 114.38      | 122.64   |
| 23  | J16   | 731  | LEU  | CA-C-N | -6.12 | 112.03      | 122.56   |
| 23  | J16   | 731  | LEU  | C-N-CA | -6.12 | 112.03      | 122.56   |
| 3   | N8    | 220  | PRO  | O-C-N  | -6.12 | 116.54      | 123.03   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 1544 | GLY  | CA-C-N | -6.12 | 112.74      | 122.29   |
| 10  | C16   | 1544 | GLY  | C-N-CA | -6.12 | 112.74      | 122.29   |
| 10  | C8    | 1277 | SER  | O-C-N  | -6.12 | 115.77      | 123.05   |
| 10  | C8    | 1544 | GLY  | CA-C-N | -6.12 | 112.74      | 122.29   |
| 10  | C8    | 1544 | GLY  | C-N-CA | -6.12 | 112.74      | 122.29   |
| 18  | B8    | 226  | TYR  | O-C-N  | 6.12  | 129.13      | 122.15   |
| 10  | C8    | 455  | GLY  | CA-C-N | -6.12 | 114.08      | 123.14   |
| 10  | C8    | 455  | GLY  | C-N-CA | -6.12 | 114.08      | 123.14   |
| 10  | C24   | 1544 | GLY  | CA-C-N | -6.12 | 112.74      | 122.29   |
| 10  | C24   | 1544 | GLY  | C-N-CA | -6.12 | 112.74      | 122.29   |
| 10  | C8    | 594  | LYS  | O-C-N  | 6.12  | 128.61      | 122.12   |
| 18  | B     | 1062 | SER  | O-C-N  | 6.12  | 130.63      | 122.43   |
| 10  | C24   | 1277 | SER  | O-C-N  | -6.12 | 115.77      | 123.05   |
| 9   | K     | 719  | GLY  | CA-C-N | 6.12  | 131.93      | 121.35   |
| 9   | K     | 719  | GLY  | C-N-CA | 6.12  | 131.93      | 121.35   |
| 18  | B8    | 1924 | GLY  | O-C-N  | -6.12 | 115.76      | 122.24   |
| 10  | C32   | 1443 | ASP  | CA-C-N | 6.11  | 133.39      | 121.41   |
| 10  | C32   | 1443 | ASP  | C-N-CA | 6.11  | 133.39      | 121.41   |
| 14  | W     | 609  | THR  | CA-C-N | 6.11  | 126.47      | 119.93   |
| 14  | W     | 609  | THR  | C-N-CA | 6.11  | 126.47      | 119.93   |
| 10  | C     | 1357 | LEU  | O-C-N  | -6.11 | 114.46      | 122.59   |
| 10  | C24   | 594  | LYS  | O-C-N  | 6.11  | 128.59      | 122.12   |
| 18  | B     | 226  | TYR  | O-C-N  | 6.11  | 129.11      | 122.15   |
| 18  | B8    | 1062 | SER  | O-C-N  | 6.11  | 130.62      | 122.43   |
| 23  | J32   | 736  | HIS  | CA-C-N | -6.11 | 112.33      | 120.63   |
| 23  | J32   | 736  | HIS  | C-N-CA | -6.11 | 112.33      | 120.63   |
| 10  | C     | 1443 | ASP  | CA-C-N | 6.10  | 133.37      | 121.41   |
| 10  | C     | 1443 | ASP  | C-N-CA | 6.10  | 133.37      | 121.41   |
| 10  | C32   | 1277 | SER  | O-C-N  | -6.10 | 115.79      | 123.05   |
| 6   | O     | 162  | THR  | O-C-N  | -6.10 | 114.47      | 122.59   |
| 6   | O8    | 162  | THR  | O-C-N  | -6.10 | 114.47      | 122.59   |
| 10  | C24   | 530  | THR  | O-C-N  | -6.10 | 114.50      | 122.43   |
| 18  | B     | 500  | THR  | CA-C-N | 6.10  | 133.19      | 121.54   |
| 18  | B     | 500  | THR  | C-N-CA | 6.10  | 133.19      | 121.54   |
| 19  | 4     | 6    | HIS  | O-C-N  | 6.10  | 128.24      | 121.53   |
| 6   | O16   | 158  | ASP  | CA-C-N | 6.10  | 132.33      | 120.99   |
| 6   | O16   | 158  | ASP  | C-N-CA | 6.10  | 132.33      | 120.99   |
| 19  | 4     | 67   | SER  | CA-C-N | -6.10 | 109.46      | 121.41   |
| 19  | 4     | 67   | SER  | C-N-CA | -6.10 | 109.46      | 121.41   |
| 6   | O     | 158  | ASP  | CA-C-N | 6.10  | 132.33      | 120.99   |
| 6   | O     | 158  | ASP  | C-N-CA | 6.10  | 132.33      | 120.99   |
| 5   | P8    | 18   | THR  | CA-C-N | -6.10 | 112.88      | 121.72   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | P8    | 18   | THR  | C-N-CA | -6.10 | 112.88      | 121.72   |
| 6   | O8    | 158  | ASP  | CA-C-N | 6.10  | 132.33      | 120.99   |
| 6   | O8    | 158  | ASP  | C-N-CA | 6.10  | 132.33      | 120.99   |
| 11  | A32   | 794  | THR  | O-C-N  | -6.09 | 115.44      | 122.93   |
| 18  | B8    | 989  | ILE  | O-C-N  | -6.09 | 114.15      | 121.10   |
| 10  | C8    | 530  | THR  | O-C-N  | -6.09 | 114.51      | 122.43   |
| 10  | C8    | 1443 | ASP  | CA-C-N | 6.09  | 133.35      | 121.41   |
| 10  | C8    | 1443 | ASP  | C-N-CA | 6.09  | 133.35      | 121.41   |
| 10  | C24   | 426  | LEU  | O-C-N  | -6.09 | 115.21      | 122.15   |
| 18  | B     | 1614 | GLU  | O-C-N  | 6.09  | 129.76      | 122.27   |
| 10  | C24   | 1443 | ASP  | CA-C-N | 6.08  | 133.34      | 121.41   |
| 10  | C24   | 1443 | ASP  | C-N-CA | 6.08  | 133.34      | 121.41   |
| 18  | B     | 795  | ASP  | CA-C-N | 6.08  | 129.56      | 120.31   |
| 18  | B     | 795  | ASP  | C-N-CA | 6.08  | 129.56      | 120.31   |
| 12  | A48   | 794  | THR  | O-C-N  | -6.08 | 115.45      | 122.93   |
| 5   | P     | 18   | THR  | CA-C-N | -6.08 | 112.90      | 121.72   |
| 5   | P     | 18   | THR  | C-N-CA | -6.08 | 112.90      | 121.72   |
| 10  | C16   | 426  | LEU  | O-C-N  | -6.08 | 115.22      | 122.15   |
| 11  | A40   | 794  | THR  | O-C-N  | -6.08 | 115.45      | 122.93   |
| 18  | B8    | 795  | ASP  | CA-C-N | 6.08  | 129.56      | 120.31   |
| 18  | B8    | 795  | ASP  | C-N-CA | 6.08  | 129.56      | 120.31   |
| 10  | C16   | 1659 | ASP  | O-C-N  | -6.08 | 115.77      | 122.09   |
| 10  | C24   | 1659 | ASP  | O-C-N  | -6.08 | 115.77      | 122.09   |
| 11  | A16   | 794  | THR  | O-C-N  | -6.08 | 115.45      | 122.93   |
| 18  | B     | 1924 | GLY  | O-C-N  | -6.08 | 115.80      | 122.24   |
| 23  | J16   | 736  | HIS  | CA-C-N | -6.07 | 112.37      | 120.63   |
| 23  | J16   | 736  | HIS  | C-N-CA | -6.07 | 112.37      | 120.63   |
| 7   | Q8    | 92   | GLY  | CA-C-N | 6.07  | 133.31      | 121.41   |
| 7   | Q8    | 92   | GLY  | C-N-CA | 6.07  | 133.31      | 121.41   |
| 7   | Q8    | 277  | ASN  | O-C-N  | 6.07  | 128.30      | 121.32   |
| 18  | B8    | 500  | THR  | CA-C-N | 6.07  | 133.13      | 121.54   |
| 18  | B8    | 500  | THR  | C-N-CA | 6.07  | 133.13      | 121.54   |
| 23  | J24   | 736  | HIS  | CA-C-N | -6.07 | 112.38      | 120.63   |
| 23  | J24   | 736  | HIS  | C-N-CA | -6.07 | 112.38      | 120.63   |
| 2   | M     | 448  | ASP  | O-C-N  | -6.07 | 114.52      | 122.59   |
| 5   | P16   | 142  | SER  | O-C-N  | -6.07 | 115.94      | 123.04   |
| 21  | H8    | 292  | LYS  | O-C-N  | -6.07 | 116.21      | 123.31   |
| 10  | C16   | 594  | LYS  | O-C-N  | 6.07  | 128.55      | 122.12   |
| 23  | J8    | 736  | HIS  | CA-C-N | -6.07 | 112.38      | 120.63   |
| 23  | J8    | 736  | HIS  | C-N-CA | -6.07 | 112.38      | 120.63   |
| 10  | C24   | 423  | SER  | O-C-N  | -6.06 | 115.56      | 123.02   |
| 18  | B8    | 1614 | GLU  | O-C-N  | 6.06  | 129.73      | 122.27   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C     | 530  | THR  | O-C-N  | -6.06 | 114.55      | 122.43   |
| 19  | 48    | 67   | SER  | CA-C-N | -6.06 | 109.53      | 121.41   |
| 19  | 48    | 67   | SER  | C-N-CA | -6.06 | 109.53      | 121.41   |
| 10  | C16   | 1250 | ALA  | O-C-N  | 6.06  | 128.54      | 122.12   |
| 7   | Q16   | 92   | GLY  | CA-C-N | 6.06  | 133.28      | 121.41   |
| 7   | Q16   | 92   | GLY  | C-N-CA | 6.06  | 133.28      | 121.41   |
| 18  | B     | 1419 | LYS  | O-C-N  | -6.06 | 114.53      | 122.59   |
| 10  | C     | 717  | GLU  | CA-C-N | -6.05 | 108.49      | 121.63   |
| 10  | C     | 717  | GLU  | C-N-CA | -6.05 | 108.49      | 121.63   |
| 10  | C16   | 1357 | LEU  | O-C-N  | -6.05 | 114.54      | 122.59   |
| 10  | C16   | 423  | SER  | O-C-N  | -6.05 | 115.58      | 123.02   |
| 10  | C8    | 423  | SER  | O-C-N  | -6.05 | 115.58      | 123.02   |
| 3   | N8    | 57   | GLY  | O-C-N  | 6.05  | 127.82      | 121.77   |
| 13  | V     | 833  | ASN  | O-C-N  | -6.05 | 114.36      | 121.32   |
| 21  | H16   | 326  | GLY  | CA-C-N | 6.05  | 133.09      | 121.54   |
| 21  | H16   | 326  | GLY  | C-N-CA | 6.05  | 133.09      | 121.54   |
| 20  | E8    | 345  | LEU  | O-C-N  | -6.04 | 114.23      | 122.33   |
| 22  | I8    | 164  | LEU  | O-C-N  | 6.04  | 129.04      | 122.15   |
| 10  | C32   | 1691 | GLU  | O-C-N  | 6.04  | 128.62      | 122.09   |
| 6   | O16   | 162  | THR  | O-C-N  | -6.04 | 114.55      | 122.59   |
| 9   | K8    | 719  | GLY  | CA-C-N | 6.04  | 131.80      | 121.35   |
| 9   | K8    | 719  | GLY  | C-N-CA | 6.04  | 131.80      | 121.35   |
| 18  | B8    | 1419 | LYS  | O-C-N  | -6.04 | 114.55      | 122.59   |
| 9   | K     | 721  | PRO  | O-C-N  | -6.04 | 114.86      | 122.17   |
| 9   | K8    | 721  | PRO  | O-C-N  | -6.04 | 114.86      | 122.17   |
| 9   | K8    | 1241 | THR  | O-C-N  | -6.04 | 114.97      | 122.82   |
| 18  | B     | 1124 | GLY  | CA-C-N | 6.04  | 132.84      | 121.97   |
| 18  | B     | 1124 | GLY  | C-N-CA | 6.04  | 132.84      | 121.97   |
| 19  | 48    | 6    | HIS  | O-C-N  | 6.03  | 128.17      | 121.53   |
| 10  | C     | 1277 | SER  | O-C-N  | -6.03 | 115.87      | 123.05   |
| 18  | B8    | 1695 | HIS  | O-C-N  | 6.03  | 129.03      | 122.15   |
| 20  | E     | 345  | LEU  | O-C-N  | -6.03 | 114.25      | 122.33   |
| 5   | P16   | 585  | VAL  | O-C-N  | 6.03  | 127.72      | 121.87   |
| 10  | C16   | 717  | GLU  | CA-C-N | -6.03 | 108.55      | 121.63   |
| 10  | C16   | 717  | GLU  | C-N-CA | -6.03 | 108.55      | 121.63   |
| 22  | I24   | 164  | LEU  | O-C-N  | 6.03  | 129.03      | 122.15   |
| 18  | B     | 1634 | LEU  | O-C-N  | -6.03 | 115.19      | 122.48   |
| 10  | C32   | 717  | GLU  | CA-C-N | -6.03 | 108.56      | 121.63   |
| 10  | C32   | 717  | GLU  | C-N-CA | -6.03 | 108.56      | 121.63   |
| 10  | C24   | 717  | GLU  | CA-C-N | -6.02 | 108.57      | 121.63   |
| 10  | C24   | 717  | GLU  | C-N-CA | -6.02 | 108.57      | 121.63   |
| 10  | C32   | 1659 | ASP  | O-C-N  | -6.02 | 115.83      | 122.09   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 14  | W     | 703  | GLY  | CA-C-N   | 6.02  | 133.03      | 121.54   |
| 14  | W     | 703  | GLY  | C-N-CA   | 6.02  | 133.03      | 121.54   |
| 3   | N16   | 57   | GLY  | O-C-N    | 6.01  | 127.78      | 121.77   |
| 9   | K     | 1049 | ASP  | CA-C-N   | -6.01 | 112.35      | 121.31   |
| 9   | K     | 1049 | ASP  | C-N-CA   | -6.01 | 112.35      | 121.31   |
| 9   | K     | 1241 | THR  | O-C-N    | -6.01 | 115.00      | 122.82   |
| 10  | C     | 1659 | ASP  | O-C-N    | -6.01 | 115.83      | 122.09   |
| 10  | C8    | 507  | SER  | O-C-N    | -6.01 | 114.91      | 122.19   |
| 18  | B8    | 1602 | SER  | O-C-N    | -6.01 | 114.59      | 122.59   |
| 11  | A40   | 781  | LEU  | O-C-N    | 6.01  | 128.16      | 121.43   |
| 23  | J8    | 685  | GLY  | O-C-N    | 6.01  | 131.27      | 121.53   |
| 22  | I24   | 95   | LEU  | CA-C-N   | -6.01 | 113.24      | 122.62   |
| 22  | I24   | 95   | LEU  | C-N-CA   | -6.01 | 113.24      | 122.62   |
| 10  | C32   | 423  | SER  | O-C-N    | -6.01 | 115.63      | 123.02   |
| 18  | B     | 989  | ILE  | O-C-N    | -6.01 | 114.25      | 121.10   |
| 18  | B     | 1602 | SER  | O-C-N    | -6.01 | 114.60      | 122.59   |
| 18  | B8    | 1073 | GLY  | O-C-N    | -6.01 | 115.81      | 122.60   |
| 18  | B8    | 1634 | LEU  | O-C-N    | -6.01 | 115.21      | 122.48   |
| 3   | N     | 57   | GLY  | O-C-N    | 6.00  | 127.77      | 121.77   |
| 10  | C24   | 1034 | SER  | O-C-N    | -6.00 | 113.67      | 122.43   |
| 18  | B8    | 1124 | GLY  | CA-C-N   | 6.00  | 132.78      | 121.97   |
| 18  | B8    | 1124 | GLY  | C-N-CA   | 6.00  | 132.78      | 121.97   |
| 12  | A48   | 781  | LEU  | O-C-N    | 6.00  | 128.16      | 121.43   |
| 5   | P8    | 8    | SER  | CA-C-N   | 6.00  | 133.17      | 121.41   |
| 5   | P8    | 8    | SER  | C-N-CA   | 6.00  | 133.17      | 121.41   |
| 21  | H8    | 326  | GLY  | CA-C-N   | 6.00  | 133.00      | 121.54   |
| 21  | H8    | 326  | GLY  | C-N-CA   | 6.00  | 133.00      | 121.54   |
| 10  | C     | 677  | GLY  | O-C-N    | -6.00 | 114.90      | 122.70   |
| 21  | H     | 326  | GLY  | CA-C-N   | 6.00  | 132.99      | 121.54   |
| 21  | H     | 326  | GLY  | C-N-CA   | 6.00  | 132.99      | 121.54   |
| 1   | R     | 356  | ASN  | CA-CB-CG | 5.99  | 118.59      | 112.60   |
| 5   | P     | 8    | SER  | CA-C-N   | 5.99  | 133.16      | 121.41   |
| 5   | P     | 8    | SER  | C-N-CA   | 5.99  | 133.16      | 121.41   |
| 10  | C16   | 507  | SER  | O-C-N    | -5.99 | 114.94      | 122.19   |
| 10  | C16   | 1034 | SER  | O-C-N    | -5.99 | 113.68      | 122.43   |
| 10  | C     | 423  | SER  | O-C-N    | -5.99 | 115.65      | 123.02   |
| 22  | I     | 95   | LEU  | CA-C-N   | -5.99 | 113.27      | 122.62   |
| 22  | I     | 95   | LEU  | C-N-CA   | -5.99 | 113.27      | 122.62   |
| 24  | D40   | 1152 | ALA  | N-CA-C   | 5.99  | 123.56      | 110.80   |
| 22  | I16   | 95   | LEU  | CA-C-N   | -5.99 | 113.28      | 122.62   |
| 22  | I16   | 95   | LEU  | C-N-CA   | -5.99 | 113.28      | 122.62   |
| 23  | J24   | 685  | GLY  | O-C-N    | 5.99  | 131.23      | 121.53   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | P16   | 8    | SER  | CA-C-N | 5.99  | 133.14      | 121.41   |
| 5   | P16   | 8    | SER  | C-N-CA | 5.99  | 133.14      | 121.41   |
| 9   | K8    | 659  | LYS  | O-C-N  | 5.99  | 128.47      | 122.12   |
| 24  | D     | 1152 | ALA  | N-CA-C | 5.99  | 123.55      | 110.80   |
| 10  | C24   | 507  | SER  | O-C-N  | -5.98 | 114.95      | 122.19   |
| 21  | H24   | 326  | GLY  | CA-C-N | 5.98  | 132.97      | 121.54   |
| 21  | H24   | 326  | GLY  | C-N-CA | 5.98  | 132.97      | 121.54   |
| 2   | M     | 432  | ARG  | O-C-N  | 5.98  | 128.97      | 122.15   |
| 10  | C16   | 1337 | LEU  | CA-C-N | -5.98 | 112.67      | 122.54   |
| 10  | C16   | 1337 | LEU  | C-N-CA | -5.98 | 112.67      | 122.54   |
| 10  | C24   | 1621 | LYS  | CA-C-N | -5.98 | 110.11      | 121.54   |
| 10  | C24   | 1621 | LYS  | C-N-CA | -5.98 | 110.11      | 121.54   |
| 22  | I16   | 164  | LEU  | O-C-N  | 5.98  | 128.97      | 122.15   |
| 23  | J16   | 685  | GLY  | O-C-N  | 5.98  | 131.22      | 121.53   |
| 24  | D32   | 1152 | ALA  | N-CA-C | 5.98  | 123.54      | 110.80   |
| 7   | Q16   | 277  | ASN  | O-C-N  | 5.98  | 128.20      | 121.32   |
| 13  | V     | 830  | GLN  | O-C-N  | -5.98 | 114.34      | 122.36   |
| 10  | C     | 507  | SER  | O-C-N  | -5.98 | 114.95      | 122.19   |
| 22  | I8    | 95   | LEU  | CA-C-N | -5.98 | 113.30      | 122.62   |
| 22  | I8    | 95   | LEU  | C-N-CA | -5.98 | 113.30      | 122.62   |
| 18  | B     | 1909 | LEU  | O-C-N  | 5.98  | 128.96      | 122.15   |
| 24  | D24   | 1152 | ALA  | N-CA-C | 5.98  | 123.53      | 110.80   |
| 24  | D8    | 1152 | ALA  | N-CA-C | 5.97  | 123.52      | 110.80   |
| 10  | C16   | 1621 | LYS  | CA-C-N | -5.97 | 110.13      | 121.54   |
| 10  | C16   | 1621 | LYS  | C-N-CA | -5.97 | 110.13      | 121.54   |
| 10  | C8    | 1621 | LYS  | CA-C-N | -5.97 | 110.13      | 121.54   |
| 10  | C8    | 1621 | LYS  | C-N-CA | -5.97 | 110.13      | 121.54   |
| 11  | A16   | 781  | LEU  | O-C-N  | 5.97  | 128.12      | 121.43   |
| 18  | B     | 1934 | LYS  | O-C-N  | 5.97  | 128.45      | 122.12   |
| 1   | R8    | 1376 | LYS  | O-C-N  | -5.97 | 113.48      | 122.20   |
| 1   | R     | 1376 | LYS  | O-C-N  | -5.97 | 113.48      | 122.20   |
| 10  | C24   | 1691 | GLU  | O-C-N  | 5.97  | 128.54      | 122.09   |
| 11  | A40   | 124  | ASN  | CA-C-N | 5.97  | 128.90      | 120.42   |
| 11  | A40   | 124  | ASN  | C-N-CA | 5.97  | 128.90      | 120.42   |
| 18  | B8    | 1418 | ALA  | CA-C-N | 5.97  | 132.94      | 121.54   |
| 18  | B8    | 1418 | ALA  | C-N-CA | 5.97  | 132.94      | 121.54   |
| 19  | 4     | 135  | GLU  | O-C-N  | 5.97  | 127.27      | 121.66   |
| 6   | O     | 224  | ASP  | O-C-N  | -5.97 | 114.97      | 122.19   |
| 18  | B     | 1418 | ALA  | CA-C-N | 5.97  | 132.94      | 121.54   |
| 18  | B     | 1418 | ALA  | C-N-CA | 5.97  | 132.94      | 121.54   |
| 10  | C32   | 1337 | LEU  | CA-C-N | -5.97 | 112.69      | 122.54   |
| 10  | C32   | 1337 | LEU  | C-N-CA | -5.97 | 112.69      | 122.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | R8    | 356  | ASN  | CA-CB-CG | 5.97  | 118.57      | 112.60   |
| 1   | R16   | 1376 | LYS  | O-C-N    | -5.97 | 113.49      | 122.20   |
| 10  | C     | 594  | LYS  | O-C-N    | 5.97  | 128.44      | 122.12   |
| 1   | R     | 1242 | SER  | O-C-N    | -5.96 | 115.02      | 122.35   |
| 10  | C8    | 1337 | LEU  | CA-C-N   | -5.96 | 112.70      | 122.54   |
| 10  | C8    | 1337 | LEU  | C-N-CA   | -5.96 | 112.70      | 122.54   |
| 5   | P8    | 585  | VAL  | O-C-N    | 5.96  | 127.65      | 121.87   |
| 12  | A     | 124  | ASN  | CA-C-N   | 5.96  | 128.88      | 120.42   |
| 12  | A     | 124  | ASN  | C-N-CA   | 5.96  | 128.88      | 120.42   |
| 18  | B     | 1695 | HIS  | O-C-N    | 5.96  | 128.95      | 122.15   |
| 23  | J32   | 685  | GLY  | O-C-N    | 5.96  | 131.19      | 121.53   |
| 12  | A48   | 124  | ASN  | CA-C-N   | 5.96  | 128.89      | 120.42   |
| 12  | A48   | 124  | ASN  | C-N-CA   | 5.96  | 128.89      | 120.42   |
| 10  | C     | 1034 | SER  | O-C-N    | -5.96 | 113.73      | 122.43   |
| 18  | B     | 1523 | ARG  | CA-C-N   | -5.96 | 112.88      | 122.24   |
| 18  | B     | 1523 | ARG  | C-N-CA   | -5.96 | 112.88      | 122.24   |
| 1   | R16   | 356  | ASN  | CA-CB-CG | 5.96  | 118.56      | 112.60   |
| 22  | I     | 164  | LEU  | O-C-N    | 5.96  | 128.94      | 122.15   |
| 24  | D16   | 1152 | ALA  | N-CA-C   | 5.96  | 123.49      | 110.80   |
| 10  | C32   | 507  | SER  | O-C-N    | -5.96 | 114.98      | 122.19   |
| 10  | C32   | 1034 | SER  | O-C-N    | -5.96 | 113.73      | 122.43   |
| 1   | R8    | 1242 | SER  | O-C-N    | -5.96 | 115.02      | 122.35   |
| 11  | A24   | 124  | ASN  | CA-C-N   | 5.96  | 128.88      | 120.42   |
| 11  | A24   | 124  | ASN  | C-N-CA   | 5.96  | 128.88      | 120.42   |
| 23  | J24   | 679  | GLU  | CA-C-N   | 5.96  | 132.92      | 121.54   |
| 23  | J24   | 679  | GLU  | C-N-CA   | 5.96  | 132.92      | 121.54   |
| 18  | B     | 599  | ILE  | CA-C-N   | 5.96  | 128.86      | 120.28   |
| 18  | B     | 599  | ILE  | C-N-CA   | 5.96  | 128.86      | 120.28   |
| 6   | O16   | 224  | ASP  | O-C-N    | -5.95 | 114.99      | 122.19   |
| 1   | R     | 801  | PHE  | CA-CB-CG | 5.95  | 119.75      | 113.80   |
| 18  | B8    | 599  | ILE  | CA-C-N   | 5.95  | 128.85      | 120.28   |
| 18  | B8    | 599  | ILE  | C-N-CA   | 5.95  | 128.85      | 120.28   |
| 16  | A8    | 124  | ASN  | CA-C-N   | 5.95  | 128.87      | 120.42   |
| 16  | A8    | 124  | ASN  | C-N-CA   | 5.95  | 128.87      | 120.42   |
| 18  | B     | 1073 | GLY  | O-C-N    | -5.95 | 115.88      | 122.60   |
| 10  | C24   | 1337 | LEU  | CA-C-N   | -5.95 | 112.73      | 122.54   |
| 10  | C24   | 1337 | LEU  | C-N-CA   | -5.95 | 112.73      | 122.54   |
| 12  | A     | 781  | LEU  | O-C-N    | 5.95  | 128.09      | 121.43   |
| 10  | C8    | 670  | GLU  | CA-C-N   | 5.95  | 134.28      | 123.27   |
| 10  | C8    | 670  | GLU  | C-N-CA   | 5.95  | 134.28      | 123.27   |
| 18  | B8    | 1934 | LYS  | O-C-N    | 5.95  | 128.43      | 122.12   |
| 19  | 48    | 135  | GLU  | O-C-N    | 5.95  | 127.25      | 121.66   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | P     | 187  | TRP  | CA-C-N | 5.95  | 128.43      | 120.58   |
| 5   | P     | 187  | TRP  | C-N-CA | 5.95  | 128.43      | 120.58   |
| 5   | P16   | 187  | TRP  | CA-C-N | 5.95  | 128.43      | 120.58   |
| 5   | P16   | 187  | TRP  | C-N-CA | 5.95  | 128.43      | 120.58   |
| 9   | K     | 1239 | ASP  | CA-C-N | 5.95  | 132.90      | 121.54   |
| 9   | K     | 1239 | ASP  | C-N-CA | 5.95  | 132.90      | 121.54   |
| 10  | C16   | 677  | GLY  | O-C-N  | -5.95 | 114.97      | 122.70   |
| 10  | C32   | 1621 | LYS  | CA-C-N | -5.95 | 110.18      | 121.54   |
| 10  | C32   | 1621 | LYS  | C-N-CA | -5.95 | 110.18      | 121.54   |
| 10  | C8    | 1034 | SER  | O-C-N  | -5.94 | 113.75      | 122.43   |
| 23  | J16   | 679  | GLU  | CA-C-N | 5.94  | 132.89      | 121.54   |
| 23  | J16   | 679  | GLU  | C-N-CA | 5.94  | 132.89      | 121.54   |
| 10  | C     | 1621 | LYS  | CA-C-N | -5.94 | 110.19      | 121.54   |
| 10  | C     | 1621 | LYS  | C-N-CA | -5.94 | 110.19      | 121.54   |
| 11  | A32   | 736  | PRO  | CA-C-N | 5.94  | 131.81      | 122.78   |
| 11  | A32   | 736  | PRO  | C-N-CA | 5.94  | 131.81      | 122.78   |
| 10  | C32   | 670  | GLU  | CA-C-N | 5.94  | 134.26      | 123.27   |
| 10  | C32   | 670  | GLU  | C-N-CA | 5.94  | 134.26      | 123.27   |
| 5   | P8    | 425  | TRP  | CA-C-N | 5.94  | 128.24      | 120.28   |
| 5   | P8    | 425  | TRP  | C-N-CA | 5.94  | 128.24      | 120.28   |
| 6   | O8    | 224  | ASP  | O-C-N  | -5.94 | 115.00      | 122.19   |
| 18  | B8    | 1523 | ARG  | CA-C-N | -5.94 | 112.92      | 122.24   |
| 18  | B8    | 1523 | ARG  | C-N-CA | -5.94 | 112.92      | 122.24   |
| 12  | A     | 736  | PRO  | CA-C-N | 5.94  | 131.81      | 122.78   |
| 12  | A     | 736  | PRO  | C-N-CA | 5.94  | 131.81      | 122.78   |
| 5   | P     | 585  | VAL  | O-C-N  | 5.94  | 127.63      | 121.87   |
| 5   | P8    | 187  | TRP  | CA-C-N | 5.94  | 128.42      | 120.58   |
| 5   | P8    | 187  | TRP  | C-N-CA | 5.94  | 128.42      | 120.58   |
| 18  | B     | 293  | PRO  | CA-C-N | 5.94  | 128.23      | 120.28   |
| 18  | B     | 293  | PRO  | C-N-CA | 5.94  | 128.23      | 120.28   |
| 9   | K     | 1281 | SER  | O-C-N  | -5.93 | 115.53      | 122.89   |
| 9   | K8    | 1049 | ASP  | CA-C-N | -5.93 | 112.47      | 121.31   |
| 9   | K8    | 1049 | ASP  | C-N-CA | -5.93 | 112.47      | 121.31   |
| 1   | R16   | 1242 | SER  | O-C-N  | -5.93 | 115.05      | 122.35   |
| 10  | C24   | 670  | GLU  | CA-C-N | 5.93  | 134.24      | 123.27   |
| 10  | C24   | 670  | GLU  | C-N-CA | 5.93  | 134.24      | 123.27   |
| 23  | J8    | 679  | GLU  | CA-C-N | 5.93  | 132.87      | 121.54   |
| 23  | J8    | 679  | GLU  | C-N-CA | 5.93  | 132.87      | 121.54   |
| 12  | A48   | 736  | PRO  | CA-C-N | 5.93  | 131.80      | 122.78   |
| 12  | A48   | 736  | PRO  | C-N-CA | 5.93  | 131.80      | 122.78   |
| 10  | C32   | 633  | SER  | CA-C-N | 5.93  | 132.87      | 121.54   |
| 10  | C32   | 633  | SER  | C-N-CA | 5.93  | 132.87      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C32   | 677  | GLY  | O-C-N  | -5.93 | 114.99      | 122.70   |
| 3   | N8    | 169  | SER  | O-C-N  | -5.93 | 115.95      | 123.06   |
| 10  | C     | 1337 | LEU  | CA-C-N | -5.93 | 112.76      | 122.54   |
| 10  | C     | 1337 | LEU  | C-N-CA | -5.93 | 112.76      | 122.54   |
| 18  | B8    | 1909 | LEU  | O-C-N  | 5.93  | 128.91      | 122.15   |
| 11  | A24   | 736  | PRO  | CA-C-N | 5.93  | 131.79      | 122.78   |
| 11  | A24   | 736  | PRO  | C-N-CA | 5.93  | 131.79      | 122.78   |
| 23  | J32   | 679  | GLU  | CA-C-N | 5.93  | 132.86      | 121.54   |
| 23  | J32   | 679  | GLU  | C-N-CA | 5.93  | 132.86      | 121.54   |
| 5   | P16   | 193  | VAL  | O-C-N  | 5.92  | 127.62      | 121.87   |
| 11  | A40   | 736  | PRO  | CA-C-N | 5.92  | 131.78      | 122.78   |
| 11  | A40   | 736  | PRO  | C-N-CA | 5.92  | 131.78      | 122.78   |
| 11  | A16   | 736  | PRO  | CA-C-N | 5.92  | 131.78      | 122.78   |
| 11  | A16   | 736  | PRO  | C-N-CA | 5.92  | 131.78      | 122.78   |
| 10  | C16   | 277  | SER  | O-C-N  | -5.92 | 115.40      | 122.15   |
| 10  | C8    | 277  | SER  | O-C-N  | -5.92 | 115.40      | 122.15   |
| 11  | A32   | 781  | LEU  | O-C-N  | 5.92  | 128.06      | 121.43   |
| 3   | N     | 169  | SER  | O-C-N  | -5.92 | 115.95      | 123.06   |
| 10  | C     | 1634 | GLN  | O-C-N  | 5.92  | 128.40      | 122.12   |
| 10  | C8    | 677  | GLY  | O-C-N  | -5.92 | 115.00      | 122.70   |
| 10  | C16   | 1491 | CYS  | CA-C-N | 5.92  | 130.07      | 120.60   |
| 10  | C16   | 1491 | CYS  | C-N-CA | 5.92  | 130.07      | 120.60   |
| 9   | K     | 1273 | GLU  | CA-C-N | 5.92  | 133.01      | 121.41   |
| 9   | K     | 1273 | GLU  | C-N-CA | 5.92  | 133.01      | 121.41   |
| 11  | A24   | 781  | LEU  | O-C-N  | 5.92  | 128.06      | 121.43   |
| 18  | B8    | 612  | GLY  | CA-C-N | 5.92  | 132.84      | 121.54   |
| 18  | B8    | 612  | GLY  | C-N-CA | 5.92  | 132.84      | 121.54   |
| 9   | K8    | 1239 | ASP  | CA-C-N | 5.92  | 132.84      | 121.54   |
| 9   | K8    | 1239 | ASP  | C-N-CA | 5.92  | 132.84      | 121.54   |
| 18  | B     | 612  | GLY  | CA-C-N | 5.92  | 132.84      | 121.54   |
| 18  | B     | 612  | GLY  | C-N-CA | 5.92  | 132.84      | 121.54   |
| 18  | B8    | 1289 | ASP  | O-C-N  | -5.92 | 114.72      | 122.59   |
| 10  | C24   | 1297 | HIS  | O-C-N  | 5.91  | 128.39      | 122.12   |
| 10  | C     | 633  | SER  | CA-C-N | 5.91  | 132.84      | 121.54   |
| 10  | C     | 633  | SER  | C-N-CA | 5.91  | 132.84      | 121.54   |
| 10  | C     | 670  | GLU  | CA-C-N | 5.91  | 134.21      | 123.27   |
| 10  | C     | 670  | GLU  | C-N-CA | 5.91  | 134.21      | 123.27   |
| 20  | E     | 430  | ALA  | CA-C-N | -5.91 | 112.27      | 121.02   |
| 20  | E     | 430  | ALA  | C-N-CA | -5.91 | 112.27      | 121.02   |
| 18  | B8    | 293  | PRO  | CA-C-N | 5.91  | 128.20      | 120.28   |
| 18  | B8    | 293  | PRO  | C-N-CA | 5.91  | 128.20      | 120.28   |
| 2   | M8    | 432  | ARG  | O-C-N  | 5.90  | 128.88      | 122.15   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | K     | 659  | LYS  | O-C-N    | 5.90  | 128.37      | 122.12   |
| 10  | C16   | 633  | SER  | CA-C-N   | 5.90  | 132.81      | 121.54   |
| 10  | C16   | 633  | SER  | C-N-CA   | 5.90  | 132.81      | 121.54   |
| 10  | C16   | 670  | GLU  | CA-C-N   | 5.90  | 134.18      | 123.27   |
| 10  | C16   | 670  | GLU  | C-N-CA   | 5.90  | 134.18      | 123.27   |
| 10  | C     | 1331 | CYS  | CA-C-N   | 5.90  | 128.77      | 120.28   |
| 10  | C     | 1331 | CYS  | C-N-CA   | 5.90  | 128.77      | 120.28   |
| 3   | N16   | 169  | SER  | O-C-N    | -5.90 | 115.98      | 123.06   |
| 5   | P     | 425  | TRP  | CA-C-N   | 5.90  | 128.18      | 120.28   |
| 5   | P     | 425  | TRP  | C-N-CA   | 5.90  | 128.18      | 120.28   |
| 10  | C     | 277  | SER  | O-C-N    | -5.90 | 115.43      | 122.15   |
| 18  | B     | 1550 | ASP  | CA-C-N   | 5.89  | 133.07      | 121.58   |
| 18  | B     | 1550 | ASP  | C-N-CA   | 5.89  | 133.07      | 121.58   |
| 10  | C8    | 1491 | CYS  | CA-C-N   | 5.89  | 130.03      | 120.60   |
| 10  | C8    | 1491 | CYS  | C-N-CA   | 5.89  | 130.03      | 120.60   |
| 20  | E8    | 430  | ALA  | CA-C-N   | -5.89 | 112.30      | 121.02   |
| 20  | E8    | 430  | ALA  | C-N-CA   | -5.89 | 112.30      | 121.02   |
| 18  | B8    | 1550 | ASP  | CA-C-N   | 5.89  | 133.07      | 121.58   |
| 18  | B8    | 1550 | ASP  | C-N-CA   | 5.89  | 133.07      | 121.58   |
| 1   | R     | 1143 | ALA  | O-C-N    | -5.89 | 112.99      | 122.41   |
| 2   | M16   | 432  | ARG  | O-C-N    | 5.89  | 128.87      | 122.15   |
| 10  | C24   | 633  | SER  | CA-C-N   | 5.89  | 132.79      | 121.54   |
| 10  | C24   | 633  | SER  | C-N-CA   | 5.89  | 132.79      | 121.54   |
| 10  | C32   | 277  | SER  | O-C-N    | -5.89 | 115.44      | 122.15   |
| 10  | C32   | 1491 | CYS  | CA-C-N   | 5.89  | 130.02      | 120.60   |
| 10  | C32   | 1491 | CYS  | C-N-CA   | 5.89  | 130.02      | 120.60   |
| 5   | P16   | 425  | TRP  | CA-C-N   | 5.89  | 128.17      | 120.28   |
| 5   | P16   | 425  | TRP  | C-N-CA   | 5.89  | 128.17      | 120.28   |
| 1   | R8    | 801  | PHE  | CA-CB-CG | 5.88  | 119.68      | 113.80   |
| 4   | T16   | 259  | ILE  | CA-C-N   | 5.88  | 126.47      | 119.94   |
| 4   | T16   | 259  | ILE  | C-N-CA   | 5.88  | 126.47      | 119.94   |
| 15  | J     | 681  | GLU  | CA-C-N   | -5.88 | 113.51      | 122.21   |
| 15  | J     | 681  | GLU  | C-N-CA   | -5.88 | 113.51      | 122.21   |
| 10  | C16   | 1802 | PRO  | CA-C-N   | 5.88  | 128.64      | 120.29   |
| 10  | C16   | 1802 | PRO  | C-N-CA   | 5.88  | 128.64      | 120.29   |
| 10  | C24   | 677  | GLY  | O-C-N    | -5.88 | 115.06      | 122.70   |
| 10  | C     | 1491 | CYS  | CA-C-N   | 5.88  | 130.00      | 120.60   |
| 10  | C     | 1491 | CYS  | C-N-CA   | 5.88  | 130.00      | 120.60   |
| 9   | K8    | 1281 | SER  | O-C-N    | -5.88 | 115.61      | 122.89   |
| 18  | B     | 1289 | ASP  | O-C-N    | -5.88 | 114.78      | 122.59   |
| 5   | P8    | 193  | VAL  | O-C-N    | 5.87  | 127.57      | 121.87   |
| 6   | O16   | 119  | ARG  | CA-C-N   | -5.87 | 113.13      | 122.29   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 6   | O16   | 119  | ARG  | C-N-CA   | -5.87 | 113.13      | 122.29   |
| 10  | C8    | 1634 | GLN  | O-C-N    | 5.87  | 128.34      | 122.12   |
| 1   | R16   | 1143 | ALA  | O-C-N    | -5.86 | 113.03      | 122.41   |
| 10  | C24   | 1545 | ARG  | O-C-N    | -5.86 | 115.28      | 122.20   |
| 1   | R8    | 1143 | ALA  | O-C-N    | -5.86 | 113.04      | 122.41   |
| 9   | K8    | 1273 | GLU  | CA-C-N   | 5.86  | 132.89      | 121.41   |
| 9   | K8    | 1273 | GLU  | C-N-CA   | 5.86  | 132.89      | 121.41   |
| 10  | C32   | 1545 | ARG  | O-C-N    | -5.86 | 115.29      | 122.20   |
| 18  | B8    | 1388 | ASP  | O-C-N    | 5.85  | 129.07      | 122.22   |
| 21  | H     | 327  | SER  | CA-C-N   | -5.85 | 113.94      | 122.65   |
| 21  | H     | 327  | SER  | C-N-CA   | -5.85 | 113.94      | 122.65   |
| 10  | C24   | 1491 | CYS  | CA-C-N   | 5.84  | 129.95      | 120.60   |
| 10  | C24   | 1491 | CYS  | C-N-CA   | 5.84  | 129.95      | 120.60   |
| 3   | N     | 164  | PRO  | O-C-N    | -5.84 | 114.75      | 122.64   |
| 1   | R16   | 801  | PHE  | CA-CB-CG | 5.84  | 119.64      | 113.80   |
| 22  | I     | 104  | ASN  | CA-C-N   | 5.84  | 129.94      | 120.60   |
| 22  | I     | 104  | ASN  | C-N-CA   | 5.84  | 129.94      | 120.60   |
| 18  | B     | 1062 | SER  | CA-C-N   | -5.84 | 112.91      | 122.54   |
| 18  | B     | 1062 | SER  | C-N-CA   | -5.84 | 112.91      | 122.54   |
| 19  | 48    | 95   | THR  | O-C-N    | 5.83  | 129.04      | 122.22   |
| 3   | N16   | 164  | PRO  | O-C-N    | -5.83 | 114.77      | 122.64   |
| 5   | P     | 193  | VAL  | O-C-N    | 5.83  | 127.52      | 121.87   |
| 10  | C24   | 187  | GLY  | O-C-N    | -5.83 | 115.12      | 122.70   |
| 10  | C8    | 1545 | ARG  | O-C-N    | -5.83 | 115.32      | 122.20   |
| 19  | 4     | 95   | THR  | O-C-N    | 5.83  | 129.04      | 122.22   |
| 21  | H16   | 327  | SER  | CA-C-N   | -5.83 | 113.96      | 122.65   |
| 21  | H16   | 327  | SER  | C-N-CA   | -5.83 | 113.96      | 122.65   |
| 9   | K     | 1271 | GLU  | CA-C-N   | -5.83 | 111.02      | 120.87   |
| 9   | K     | 1271 | GLU  | C-N-CA   | -5.83 | 111.02      | 120.87   |
| 9   | K8    | 1271 | GLU  | O-C-N    | -5.83 | 114.84      | 122.59   |
| 10  | C16   | 1545 | ARG  | O-C-N    | -5.83 | 115.33      | 122.20   |
| 10  | C32   | 187  | GLY  | O-C-N    | -5.83 | 115.12      | 122.70   |
| 11  | A24   | 25   | ALA  | CA-C-N   | -5.83 | 112.58      | 119.05   |
| 11  | A24   | 25   | ALA  | C-N-CA   | -5.83 | 112.58      | 119.05   |
| 11  | A40   | 25   | ALA  | CA-C-N   | -5.83 | 112.58      | 119.05   |
| 11  | A40   | 25   | ALA  | C-N-CA   | -5.83 | 112.58      | 119.05   |
| 18  | B     | 1758 | GLU  | O-C-N    | 5.83  | 129.43      | 122.27   |
| 9   | K8    | 1271 | GLU  | CA-C-N   | -5.82 | 111.03      | 120.87   |
| 9   | K8    | 1271 | GLU  | C-N-CA   | -5.82 | 111.03      | 120.87   |
| 18  | B8    | 1062 | SER  | CA-C-N   | -5.82 | 112.93      | 122.54   |
| 18  | B8    | 1062 | SER  | C-N-CA   | -5.82 | 112.93      | 122.54   |
| 22  | I24   | 104  | ASN  | CA-C-N   | 5.82  | 129.92      | 120.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22  | I24   | 104  | ASN  | C-N-CA   | 5.82  | 129.92      | 120.60   |
| 6   | O8    | 119  | ARG  | CA-C-N   | -5.82 | 113.21      | 122.29   |
| 6   | O8    | 119  | ARG  | C-N-CA   | -5.82 | 113.21      | 122.29   |
| 10  | C24   | 277  | SER  | O-C-N    | -5.82 | 115.52      | 122.15   |
| 3   | N8    | 164  | PRO  | O-C-N    | -5.82 | 114.79      | 122.64   |
| 9   | K8    | 591  | LEU  | O-C-N    | 5.82  | 128.29      | 122.12   |
| 10  | C16   | 187  | GLY  | O-C-N    | -5.82 | 115.14      | 122.70   |
| 19  | 4     | 24   | ASN  | O-C-N    | 5.82  | 130.02      | 123.27   |
| 8   | L8    | 839  | ASP  | CA-CB-CG | 5.82  | 118.42      | 112.60   |
| 10  | C24   | 728  | SER  | CA-C-N   | 5.82  | 132.65      | 121.54   |
| 10  | C24   | 728  | SER  | C-N-CA   | 5.82  | 132.65      | 121.54   |
| 21  | H     | 245  | GLN  | O-C-N    | 5.82  | 128.78      | 122.15   |
| 21  | H8    | 327  | SER  | CA-C-N   | -5.81 | 113.99      | 122.65   |
| 21  | H8    | 327  | SER  | C-N-CA   | -5.81 | 113.99      | 122.65   |
| 10  | C     | 1802 | PRO  | CA-C-N   | 5.81  | 128.54      | 120.29   |
| 10  | C     | 1802 | PRO  | C-N-CA   | 5.81  | 128.54      | 120.29   |
| 6   | O     | 119  | ARG  | CA-C-N   | -5.81 | 113.22      | 122.29   |
| 6   | O     | 119  | ARG  | C-N-CA   | -5.81 | 113.22      | 122.29   |
| 18  | B8    | 1407 | GLN  | O-C-N    | 5.81  | 128.28      | 122.12   |
| 11  | A24   | 339  | GLN  | CA-C-N   | -5.81 | 114.40      | 120.38   |
| 11  | A24   | 339  | GLN  | C-N-CA   | -5.81 | 114.40      | 120.38   |
| 14  | W     | 592  | ALA  | CA-C-N   | 5.81  | 130.99      | 121.87   |
| 14  | W     | 592  | ALA  | C-N-CA   | 5.81  | 130.99      | 121.87   |
| 10  | C8    | 1772 | ASP  | CA-C-N   | 5.81  | 132.63      | 121.54   |
| 10  | C8    | 1772 | ASP  | C-N-CA   | 5.81  | 132.63      | 121.54   |
| 10  | C8    | 1037 | SER  | O-C-N    | -5.81 | 115.88      | 122.97   |
| 11  | A16   | 339  | GLN  | CA-C-N   | -5.81 | 114.40      | 120.38   |
| 11  | A16   | 339  | GLN  | C-N-CA   | -5.81 | 114.40      | 120.38   |
| 10  | C     | 187  | GLY  | O-C-N    | -5.80 | 115.16      | 122.70   |
| 10  | C32   | 1634 | GLN  | O-C-N    | 5.80  | 128.27      | 122.12   |
| 4   | T     | 259  | ILE  | CA-C-N   | 5.80  | 126.38      | 119.94   |
| 4   | T     | 259  | ILE  | C-N-CA   | 5.80  | 126.38      | 119.94   |
| 10  | C16   | 455  | GLY  | CA-C-N   | -5.80 | 114.12      | 123.23   |
| 10  | C16   | 455  | GLY  | C-N-CA   | -5.80 | 114.12      | 123.23   |
| 10  | C24   | 1787 | SER  | O-C-N    | -5.80 | 114.65      | 122.43   |
| 22  | I8    | 104  | ASN  | CA-C-N   | 5.80  | 129.88      | 120.60   |
| 22  | I8    | 104  | ASN  | C-N-CA   | 5.80  | 129.88      | 120.60   |
| 8   | L     | 839  | ASP  | CA-CB-CG | 5.80  | 118.40      | 112.60   |
| 21  | H24   | 327  | SER  | CA-C-N   | -5.80 | 114.01      | 122.65   |
| 21  | H24   | 327  | SER  | C-N-CA   | -5.80 | 114.01      | 122.65   |
| 10  | C8    | 187  | GLY  | O-C-N    | -5.80 | 115.17      | 122.70   |
| 10  | C8    | 1802 | PRO  | CA-C-N   | 5.80  | 128.52      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1802 | PRO  | C-N-CA | 5.80  | 128.52      | 120.29   |
| 18  | B     | 1756 | LYS  | O-C-N  | 5.80  | 128.04      | 122.07   |
| 11  | A40   | 339  | GLN  | CA-C-N | -5.79 | 114.41      | 120.38   |
| 11  | A40   | 339  | GLN  | C-N-CA | -5.79 | 114.41      | 120.38   |
| 4   | T8    | 259  | ILE  | CA-C-N | 5.79  | 126.37      | 119.94   |
| 4   | T8    | 259  | ILE  | C-N-CA | 5.79  | 126.37      | 119.94   |
| 7   | Q8    | 86   | ALA  | O-C-N  | -5.79 | 114.52      | 122.46   |
| 10  | C32   | 1802 | PRO  | CA-C-N | 5.79  | 128.52      | 120.29   |
| 10  | C32   | 1802 | PRO  | C-N-CA | 5.79  | 128.52      | 120.29   |
| 19  | 4     | 90   | GLN  | O-C-N  | -5.79 | 114.66      | 121.32   |
| 1   | R     | 1141 | GLU  | O-C-N  | -5.79 | 114.14      | 122.36   |
| 7   | Q     | 32   | ASN  | CA-C-N | -5.79 | 114.94      | 123.05   |
| 7   | Q     | 32   | ASN  | C-N-CA | -5.79 | 114.94      | 123.05   |
| 18  | B     | 1388 | ASP  | O-C-N  | 5.79  | 129.00      | 122.22   |
| 21  | H8    | 245  | GLN  | O-C-N  | 5.79  | 128.75      | 122.15   |
| 18  | B8    | 1599 | THR  | CA-C-N | -5.79 | 111.51      | 120.31   |
| 18  | B8    | 1599 | THR  | C-N-CA | -5.79 | 111.51      | 120.31   |
| 5   | P16   | 577  | SER  | O-C-N  | 5.79  | 129.39      | 122.27   |
| 11  | A32   | 25   | ALA  | CA-C-N | -5.79 | 112.63      | 119.05   |
| 11  | A32   | 25   | ALA  | C-N-CA | -5.79 | 112.63      | 119.05   |
| 10  | C24   | 1452 | GLN  | O-C-N  | 5.78  | 128.74      | 122.15   |
| 22  | I16   | 104  | ASN  | CA-C-N | 5.78  | 129.85      | 120.60   |
| 22  | I16   | 104  | ASN  | C-N-CA | 5.78  | 129.85      | 120.60   |
| 24  | D8    | 758  | ALA  | CA-C-N | 5.78  | 132.58      | 121.54   |
| 24  | D8    | 758  | ALA  | C-N-CA | 5.78  | 132.58      | 121.54   |
| 5   | P     | 260  | GLN  | CA-C-N | 5.78  | 128.03      | 120.28   |
| 5   | P     | 260  | GLN  | C-N-CA | 5.78  | 128.03      | 120.28   |
| 9   | K     | 591  | LEU  | O-C-N  | 5.78  | 128.25      | 122.12   |
| 19  | 48    | 24   | ASN  | O-C-N  | 5.78  | 129.97      | 123.27   |
| 23  | J32   | 725  | SER  | CA-C-N | 5.78  | 132.74      | 121.41   |
| 23  | J32   | 725  | SER  | C-N-CA | 5.78  | 132.74      | 121.41   |
| 5   | P16   | 260  | GLN  | CA-C-N | 5.78  | 128.02      | 120.28   |
| 5   | P16   | 260  | GLN  | C-N-CA | 5.78  | 128.02      | 120.28   |
| 9   | K8    | 1053 | MET  | CA-C-N | -5.78 | 110.51      | 121.54   |
| 9   | K8    | 1053 | MET  | C-N-CA | -5.78 | 110.51      | 121.54   |
| 10  | C24   | 147  | LEU  | O-C-N  | -5.78 | 116.59      | 123.06   |
| 18  | B     | 1599 | THR  | CA-C-N | -5.78 | 111.53      | 120.31   |
| 18  | B     | 1599 | THR  | C-N-CA | -5.78 | 111.53      | 120.31   |
| 23  | J8    | 725  | SER  | CA-C-N | 5.78  | 132.73      | 121.41   |
| 23  | J8    | 725  | SER  | C-N-CA | 5.78  | 132.73      | 121.41   |
| 9   | K     | 1271 | GLU  | O-C-N  | -5.78 | 114.91      | 122.59   |
| 9   | K8    | 1029 | VAL  | O-C-N  | 5.78  | 127.70      | 121.87   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 21  | H16   | 245  | GLN  | O-C-N  | 5.78  | 128.74      | 122.15   |
| 24  | D40   | 758  | ALA  | CA-C-N | 5.78  | 132.57      | 121.54   |
| 24  | D40   | 758  | ALA  | C-N-CA | 5.78  | 132.57      | 121.54   |
| 10  | C24   | 1802 | PRO  | CA-C-N | 5.77  | 128.49      | 120.29   |
| 10  | C24   | 1802 | PRO  | C-N-CA | 5.77  | 128.49      | 120.29   |
| 10  | C24   | 1037 | SER  | O-C-N  | -5.77 | 115.93      | 122.97   |
| 10  | C24   | 1634 | GLN  | O-C-N  | 5.77  | 128.24      | 122.12   |
| 7   | Q     | 86   | ALA  | O-C-N  | -5.77 | 114.55      | 122.46   |
| 10  | C16   | 1787 | SER  | O-C-N  | -5.77 | 114.70      | 122.43   |
| 10  | C     | 1772 | ASP  | CA-C-N | 5.77  | 132.56      | 121.54   |
| 10  | C     | 1772 | ASP  | C-N-CA | 5.77  | 132.56      | 121.54   |
| 10  | C     | 1787 | SER  | O-C-N  | -5.77 | 114.70      | 122.43   |
| 20  | E     | 447  | ILE  | O-C-N  | -5.77 | 115.36      | 122.57   |
| 24  | D16   | 758  | ALA  | CA-C-N | 5.77  | 132.56      | 121.54   |
| 24  | D16   | 758  | ALA  | C-N-CA | 5.77  | 132.56      | 121.54   |
| 10  | C     | 1037 | SER  | O-C-N  | -5.77 | 115.93      | 122.97   |
| 10  | C8    | 1060 | ALA  | CA-C-N | 5.76  | 132.55      | 121.54   |
| 10  | C8    | 1060 | ALA  | C-N-CA | 5.76  | 132.55      | 121.54   |
| 10  | C8    | 1297 | HIS  | O-C-N  | 5.76  | 128.23      | 122.12   |
| 10  | C8    | 1787 | SER  | O-C-N  | -5.76 | 114.71      | 122.43   |
| 5   | P     | 446  | HIS  | O-C-N  | 5.76  | 129.11      | 122.25   |
| 5   | P8    | 260  | GLN  | CA-C-N | 5.76  | 128.00      | 120.28   |
| 5   | P8    | 260  | GLN  | C-N-CA | 5.76  | 128.00      | 120.28   |
| 5   | P8    | 577  | SER  | O-C-N  | 5.76  | 129.36      | 122.27   |
| 23  | J8    | 727  | GLY  | O-C-N  | 5.76  | 127.72      | 122.19   |
| 10  | C32   | 1772 | ASP  | CA-C-N | 5.76  | 132.54      | 121.54   |
| 10  | C32   | 1772 | ASP  | C-N-CA | 5.76  | 132.54      | 121.54   |
| 5   | P16   | 446  | HIS  | O-C-N  | 5.76  | 129.10      | 122.25   |
| 18  | B8    | 235  | ARG  | O-C-N  | 5.76  | 128.22      | 122.12   |
| 10  | C16   | 1037 | SER  | O-C-N  | -5.76 | 115.94      | 122.97   |
| 10  | C     | 1060 | ALA  | CA-C-N | 5.76  | 132.54      | 121.54   |
| 10  | C     | 1060 | ALA  | C-N-CA | 5.76  | 132.54      | 121.54   |
| 7   | Q8    | 32   | ASN  | CA-C-N | -5.76 | 114.99      | 123.05   |
| 7   | Q8    | 32   | ASN  | C-N-CA | -5.76 | 114.99      | 123.05   |
| 10  | C16   | 1297 | HIS  | O-C-N  | 5.76  | 128.22      | 122.12   |
| 23  | J24   | 725  | SER  | CA-C-N | 5.76  | 132.69      | 121.41   |
| 23  | J24   | 725  | SER  | C-N-CA | 5.76  | 132.69      | 121.41   |
| 11  | A16   | 25   | ALA  | CA-C-N | -5.75 | 112.66      | 119.05   |
| 11  | A16   | 25   | ALA  | C-N-CA | -5.75 | 112.66      | 119.05   |
| 21  | H24   | 245  | GLN  | O-C-N  | 5.75  | 128.71      | 122.15   |
| 24  | D24   | 758  | ALA  | CA-C-N | 5.75  | 132.53      | 121.54   |
| 24  | D24   | 758  | ALA  | C-N-CA | 5.75  | 132.53      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 716  | ALA  | CA-C-N | 5.75  | 128.46      | 120.29   |
| 9   | K     | 716  | ALA  | C-N-CA | 5.75  | 128.46      | 120.29   |
| 19  | 48    | 90   | GLN  | O-C-N  | -5.75 | 114.70      | 121.32   |
| 10  | C32   | 147  | LEU  | O-C-N  | -5.75 | 116.62      | 123.06   |
| 18  | B8    | 855  | GLY  | CA-C-N | 5.75  | 135.83      | 121.80   |
| 18  | B8    | 855  | GLY  | C-N-CA | 5.75  | 135.83      | 121.80   |
| 9   | K8    | 821  | PRO  | CA-C-N | -5.75 | 113.62      | 119.83   |
| 9   | K8    | 821  | PRO  | C-N-CA | -5.75 | 113.62      | 119.83   |
| 10  | C16   | 728  | SER  | CA-C-N | 5.75  | 132.52      | 121.54   |
| 10  | C16   | 728  | SER  | C-N-CA | 5.75  | 132.52      | 121.54   |
| 23  | J16   | 725  | SER  | CA-C-N | 5.75  | 132.68      | 121.41   |
| 23  | J16   | 725  | SER  | C-N-CA | 5.75  | 132.68      | 121.41   |
| 24  | D32   | 758  | ALA  | CA-C-N | 5.75  | 132.52      | 121.54   |
| 24  | D32   | 758  | ALA  | C-N-CA | 5.75  | 132.52      | 121.54   |
| 12  | A48   | 140  | TRP  | CA-C-N | 5.75  | 128.45      | 120.29   |
| 12  | A48   | 140  | TRP  | C-N-CA | 5.75  | 128.45      | 120.29   |
| 5   | P8    | 446  | HIS  | O-C-N  | 5.75  | 129.09      | 122.25   |
| 10  | C24   | 880  | GLU  | CA-C-N | -5.75 | 113.39      | 121.72   |
| 10  | C24   | 880  | GLU  | C-N-CA | -5.75 | 113.39      | 121.72   |
| 10  | C     | 147  | LEU  | O-C-N  | -5.75 | 116.63      | 123.06   |
| 18  | B     | 1407 | GLN  | O-C-N  | 5.75  | 128.21      | 122.12   |
| 1   | R8    | 1141 | GLU  | O-C-N  | -5.74 | 114.20      | 122.36   |
| 12  | A48   | 339  | GLN  | CA-C-N | -5.74 | 114.46      | 120.38   |
| 12  | A48   | 339  | GLN  | C-N-CA | -5.74 | 114.46      | 120.38   |
| 10  | C16   | 1238 | SER  | O-C-N  | 5.74  | 128.21      | 122.12   |
| 1   | R16   | 1141 | GLU  | O-C-N  | -5.74 | 114.21      | 122.36   |
| 5   | P16   | 652  | LEU  | O-C-N  | 5.74  | 128.21      | 122.12   |
| 24  | D     | 758  | ALA  | CA-C-N | 5.74  | 132.50      | 121.54   |
| 24  | D     | 758  | ALA  | C-N-CA | 5.74  | 132.50      | 121.54   |
| 10  | C16   | 1279 | THR  | O-C-N  | -5.74 | 116.79      | 123.27   |
| 10  | C8    | 106  | GLY  | O-C-N  | -5.74 | 115.24      | 122.70   |
| 10  | C32   | 1279 | THR  | O-C-N  | -5.74 | 116.79      | 123.27   |
| 9   | K     | 1053 | MET  | CA-C-N | -5.74 | 110.59      | 121.54   |
| 9   | K     | 1053 | MET  | C-N-CA | -5.74 | 110.59      | 121.54   |
| 18  | B     | 33   | PRO  | CA-C-N | 5.74  | 127.26      | 120.09   |
| 18  | B     | 33   | PRO  | C-N-CA | 5.74  | 127.26      | 120.09   |
| 20  | E8    | 424  | GLN  | O-C-N  | -5.74 | 116.16      | 122.07   |
| 7   | Q16   | 32   | ASN  | CA-C-N | -5.73 | 115.02      | 123.05   |
| 7   | Q16   | 32   | ASN  | C-N-CA | -5.73 | 115.02      | 123.05   |
| 10  | C8    | 147  | LEU  | O-C-N  | -5.73 | 116.64      | 123.06   |
| 18  | B     | 855  | GLY  | CA-C-N | 5.73  | 135.79      | 121.80   |
| 18  | B     | 855  | GLY  | C-N-CA | 5.73  | 135.79      | 121.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10  | C24   | 1060 | ALA  | CA-C-N   | 5.73  | 132.49      | 121.54   |
| 10  | C24   | 1060 | ALA  | C-N-CA   | 5.73  | 132.49      | 121.54   |
| 14  | W     | 518  | GLU  | N-CA-C   | 5.73  | 119.47      | 111.90   |
| 1   | R8    | 304  | ASP  | CA-CB-CG | 5.73  | 118.33      | 112.60   |
| 8   | L16   | 839  | ASP  | CA-CB-CG | 5.73  | 118.33      | 112.60   |
| 11  | A24   | 140  | TRP  | CA-C-N   | 5.73  | 128.42      | 120.29   |
| 11  | A24   | 140  | TRP  | C-N-CA   | 5.73  | 128.42      | 120.29   |
| 24  | D16   | 1066 | VAL  | CA-C-N   | 5.73  | 132.48      | 121.54   |
| 24  | D16   | 1066 | VAL  | C-N-CA   | 5.73  | 132.48      | 121.54   |
| 10  | C32   | 1787 | SER  | O-C-N    | -5.73 | 114.75      | 122.43   |
| 10  | C16   | 1060 | ALA  | CA-C-N   | 5.73  | 132.48      | 121.54   |
| 10  | C16   | 1060 | ALA  | C-N-CA   | 5.73  | 132.48      | 121.54   |
| 10  | C16   | 1131 | GLY  | CA-C-N   | -5.72 | 112.74      | 120.87   |
| 10  | C16   | 1131 | GLY  | C-N-CA   | -5.72 | 112.74      | 120.87   |
| 10  | C24   | 728  | SER  | O-C-N    | -5.72 | 115.40      | 123.01   |
| 10  | C24   | 1772 | ASP  | CA-C-N   | 5.72  | 132.47      | 121.54   |
| 10  | C24   | 1772 | ASP  | C-N-CA   | 5.72  | 132.47      | 121.54   |
| 1   | R16   | 304  | ASP  | CA-CB-CG | 5.72  | 118.32      | 112.60   |
| 10  | C16   | 1772 | ASP  | CA-C-N   | 5.72  | 132.46      | 121.54   |
| 10  | C16   | 1772 | ASP  | C-N-CA   | 5.72  | 132.46      | 121.54   |
| 10  | C     | 1272 | GLN  | CA-C-N   | -5.72 | 110.20      | 121.41   |
| 10  | C     | 1272 | GLN  | C-N-CA   | -5.72 | 110.20      | 121.41   |
| 7   | Q16   | 303  | LEU  | O-C-N    | 5.72  | 127.83      | 121.43   |
| 10  | C32   | 728  | SER  | CA-C-N   | 5.72  | 132.46      | 121.54   |
| 10  | C32   | 728  | SER  | C-N-CA   | 5.72  | 132.46      | 121.54   |
| 11  | A32   | 339  | GLN  | CA-C-N   | -5.71 | 114.49      | 120.38   |
| 11  | A32   | 339  | GLN  | C-N-CA   | -5.71 | 114.49      | 120.38   |
| 10  | C32   | 1238 | SER  | O-C-N    | 5.71  | 128.18      | 122.12   |
| 10  | C32   | 1297 | HIS  | O-C-N    | 5.71  | 128.18      | 122.12   |
| 9   | K     | 821  | PRO  | CA-C-N   | -5.71 | 113.66      | 119.83   |
| 9   | K     | 821  | PRO  | C-N-CA   | -5.71 | 113.66      | 119.83   |
| 18  | B8    | 33   | PRO  | CA-C-N   | 5.71  | 127.23      | 120.09   |
| 18  | B8    | 33   | PRO  | C-N-CA   | 5.71  | 127.23      | 120.09   |
| 11  | A16   | 468  | VAL  | O-C-N    | -5.71 | 115.43      | 122.57   |
| 22  | I24   | 129  | GLU  | CA-C-N   | 5.71  | 127.93      | 120.28   |
| 22  | I24   | 129  | GLU  | C-N-CA   | 5.71  | 127.93      | 120.28   |
| 9   | K8    | 716  | ALA  | CA-C-N   | 5.71  | 128.39      | 120.29   |
| 9   | K8    | 716  | ALA  | C-N-CA   | 5.71  | 128.39      | 120.29   |
| 16  | A8    | 140  | TRP  | CA-C-N   | 5.71  | 128.39      | 120.29   |
| 16  | A8    | 140  | TRP  | C-N-CA   | 5.71  | 128.39      | 120.29   |
| 18  | B8    | 613  | LYS  | CA-C-N   | -5.71 | 110.64      | 121.54   |
| 18  | B8    | 613  | LYS  | C-N-CA   | -5.71 | 110.64      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 20  | E8    | 447  | ILE  | O-C-N  | -5.71 | 115.44      | 122.57   |
| 22  | I16   | 129  | GLU  | CA-C-N | 5.71  | 127.93      | 120.28   |
| 22  | I16   | 129  | GLU  | C-N-CA | 5.71  | 127.93      | 120.28   |
| 10  | C32   | 1037 | SER  | O-C-N  | -5.71 | 116.01      | 122.97   |
| 10  | C     | 1131 | GLY  | CA-C-N | -5.71 | 112.77      | 120.87   |
| 10  | C     | 1131 | GLY  | C-N-CA | -5.71 | 112.77      | 120.87   |
| 10  | C     | 1297 | HIS  | O-C-N  | 5.71  | 128.17      | 122.12   |
| 7   | Q16   | 86   | ALA  | O-C-N  | -5.70 | 114.65      | 122.46   |
| 10  | C16   | 1634 | GLN  | O-C-N  | 5.70  | 128.16      | 122.12   |
| 10  | C24   | 1131 | GLY  | CA-C-N | -5.70 | 112.77      | 120.87   |
| 10  | C24   | 1131 | GLY  | C-N-CA | -5.70 | 112.77      | 120.87   |
| 11  | A40   | 140  | TRP  | CA-C-N | 5.70  | 128.39      | 120.29   |
| 11  | A40   | 140  | TRP  | C-N-CA | 5.70  | 128.39      | 120.29   |
| 10  | C     | 632  | GLN  | O-C-N  | -5.70 | 115.77      | 122.96   |
| 10  | C8    | 861  | ILE  | CA-C-N | 5.70  | 130.22      | 122.07   |
| 10  | C8    | 861  | ILE  | C-N-CA | 5.70  | 130.22      | 122.07   |
| 10  | C8    | 1238 | SER  | O-C-N  | 5.70  | 128.17      | 122.12   |
| 22  | I8    | 108  | LYS  | CA-C-N | 5.70  | 128.19      | 120.38   |
| 22  | I8    | 108  | LYS  | C-N-CA | 5.70  | 128.19      | 120.38   |
| 10  | C32   | 1272 | GLN  | CA-C-N | -5.70 | 110.23      | 121.41   |
| 10  | C32   | 1272 | GLN  | C-N-CA | -5.70 | 110.23      | 121.41   |
| 10  | C8    | 1131 | GLY  | CA-C-N | -5.70 | 112.78      | 120.87   |
| 10  | C8    | 1131 | GLY  | C-N-CA | -5.70 | 112.78      | 120.87   |
| 18  | B8    | 435  | CYS  | O-C-N  | 5.70  | 128.16      | 122.12   |
| 20  | E     | 424  | GLN  | O-C-N  | -5.70 | 116.20      | 122.07   |
| 23  | J32   | 727  | GLY  | O-C-N  | 5.70  | 127.66      | 122.19   |
| 2   | M8    | 702  | VAL  | CA-C-N | 5.70  | 127.92      | 120.28   |
| 2   | M8    | 702  | VAL  | C-N-CA | 5.70  | 127.92      | 120.28   |
| 10  | C16   | 880  | GLU  | CA-C-N | -5.70 | 113.46      | 121.72   |
| 10  | C16   | 880  | GLU  | C-N-CA | -5.70 | 113.46      | 121.72   |
| 10  | C     | 415  | SER  | O-C-N  | 5.70  | 128.65      | 122.15   |
| 10  | C8    | 415  | SER  | O-C-N  | 5.70  | 128.65      | 122.15   |
| 9   | K     | 729  | VAL  | CA-C-N | 5.70  | 130.45      | 121.56   |
| 9   | K     | 729  | VAL  | C-N-CA | 5.70  | 130.45      | 121.56   |
| 10  | C16   | 415  | SER  | O-C-N  | 5.70  | 128.65      | 122.15   |
| 10  | C     | 1355 | GLU  | CA-C-N | 5.70  | 132.42      | 121.54   |
| 10  | C     | 1355 | GLU  | C-N-CA | 5.70  | 132.42      | 121.54   |
| 10  | C16   | 106  | GLY  | O-C-N  | -5.70 | 115.30      | 122.70   |
| 10  | C16   | 1272 | GLN  | CA-C-N | -5.70 | 110.25      | 121.41   |
| 10  | C16   | 1272 | GLN  | C-N-CA | -5.70 | 110.25      | 121.41   |
| 10  | C8    | 1272 | GLN  | CA-C-N | -5.70 | 110.25      | 121.41   |
| 10  | C8    | 1272 | GLN  | C-N-CA | -5.70 | 110.25      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | C32   | 1131 | GLY  | CA-C-N  | -5.70 | 112.78      | 120.87   |
| 10  | C32   | 1131 | GLY  | C-N-CA  | -5.70 | 112.78      | 120.87   |
| 5   | P16   | 15   | LEU  | O-C-N   | -5.69 | 115.71      | 122.20   |
| 9   | K     | 1239 | ASP  | O-C-N   | -5.69 | 115.42      | 122.82   |
| 12  | A     | 339  | GLN  | CA-C-N  | -5.69 | 114.52      | 120.38   |
| 12  | A     | 339  | GLN  | C-N-CA  | -5.69 | 114.52      | 120.38   |
| 8   | L16   | 717  | PRO  | N-CA-CB | 5.69  | 106.38      | 103.19   |
| 10  | C     | 1238 | SER  | O-C-N   | 5.69  | 128.15      | 122.12   |
| 10  | C8    | 880  | GLU  | CA-C-N  | -5.69 | 113.47      | 121.72   |
| 10  | C8    | 880  | GLU  | C-N-CA  | -5.69 | 113.47      | 121.72   |
| 18  | B     | 973  | ASP  | CA-C-N  | -5.69 | 113.04      | 120.44   |
| 18  | B     | 973  | ASP  | C-N-CA  | -5.69 | 113.04      | 120.44   |
| 20  | E8    | 343  | THR  | C-N-CD  | -5.69 | 101.66      | 125.00   |
| 5   | P16   | 442  | GLU  | O-C-N   | 5.69  | 128.64      | 122.15   |
| 9   | K8    | 729  | VAL  | CA-C-N  | 5.69  | 130.44      | 121.56   |
| 9   | K8    | 729  | VAL  | C-N-CA  | 5.69  | 130.44      | 121.56   |
| 10  | C16   | 728  | SER  | O-C-N   | -5.69 | 115.44      | 123.01   |
| 22  | I24   | 143  | LEU  | CA-C-N  | -5.69 | 113.30      | 122.23   |
| 22  | I24   | 143  | LEU  | C-N-CA  | -5.69 | 113.30      | 122.23   |
| 5   | P     | 442  | GLU  | O-C-N   | 5.69  | 128.63      | 122.15   |
| 7   | Q8    | 303  | LEU  | O-C-N   | 5.69  | 127.80      | 121.43   |
| 10  | C     | 880  | GLU  | CA-C-N  | -5.69 | 113.47      | 121.72   |
| 10  | C     | 880  | GLU  | C-N-CA  | -5.69 | 113.47      | 121.72   |
| 18  | B8    | 1756 | LYS  | O-C-N   | 5.69  | 127.93      | 122.07   |
| 22  | I     | 143  | LEU  | CA-C-N  | -5.69 | 113.30      | 122.23   |
| 22  | I     | 143  | LEU  | C-N-CA  | -5.69 | 113.30      | 122.23   |
| 10  | C32   | 1060 | ALA  | CA-C-N  | 5.69  | 132.40      | 121.54   |
| 10  | C32   | 1060 | ALA  | C-N-CA  | 5.69  | 132.40      | 121.54   |
| 10  | C32   | 1355 | GLU  | CA-C-N  | 5.69  | 132.40      | 121.54   |
| 10  | C32   | 1355 | GLU  | C-N-CA  | 5.69  | 132.40      | 121.54   |
| 22  | I16   | 143  | LEU  | CA-C-N  | -5.69 | 113.30      | 122.23   |
| 22  | I16   | 143  | LEU  | C-N-CA  | -5.69 | 113.30      | 122.23   |
| 10  | C     | 289  | ASP  | CA-C-N  | 5.68  | 127.89      | 120.28   |
| 10  | C     | 289  | ASP  | C-N-CA  | 5.68  | 127.89      | 120.28   |
| 10  | C     | 1336 | ALA  | CA-C-N  | 5.68  | 132.39      | 121.54   |
| 10  | C     | 1336 | ALA  | C-N-CA  | 5.68  | 132.39      | 121.54   |
| 20  | E8    | 437  | SER  | CA-C-N  | -5.68 | 110.69      | 121.54   |
| 20  | E8    | 437  | SER  | C-N-CA  | -5.68 | 110.69      | 121.54   |
| 20  | E     | 343  | THR  | C-N-CD  | -5.68 | 101.71      | 125.00   |
| 22  | I8    | 143  | LEU  | CA-C-N  | -5.68 | 113.31      | 122.23   |
| 22  | I8    | 143  | LEU  | C-N-CA  | -5.68 | 113.31      | 122.23   |
| 9   | K8    | 864  | ILE  | O-C-N   | 5.68  | 127.68      | 121.83   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10  | C24   | 1238 | SER  | O-C-N    | 5.68  | 128.14      | 122.12   |
| 10  | C8    | 1475 | GLY  | O-C-N    | 5.68  | 127.63      | 122.18   |
| 9   | K     | 864  | ILE  | O-C-N    | 5.68  | 127.68      | 121.83   |
| 18  | B     | 613  | LYS  | CA-C-N   | -5.68 | 110.70      | 121.54   |
| 18  | B     | 613  | LYS  | C-N-CA   | -5.68 | 110.70      | 121.54   |
| 20  | E     | 437  | SER  | CA-C-N   | -5.68 | 110.70      | 121.54   |
| 20  | E     | 437  | SER  | C-N-CA   | -5.68 | 110.70      | 121.54   |
| 23  | J16   | 727  | GLY  | O-C-N    | 5.68  | 127.64      | 122.19   |
| 2   | M16   | 702  | VAL  | CA-C-N   | 5.67  | 127.88      | 120.28   |
| 2   | M16   | 702  | VAL  | C-N-CA   | 5.67  | 127.88      | 120.28   |
| 9   | K     | 1090 | ASP  | O-C-N    | -5.67 | 116.31      | 123.01   |
| 10  | C24   | 1272 | GLN  | CA-C-N   | -5.67 | 110.29      | 121.41   |
| 10  | C24   | 1272 | GLN  | C-N-CA   | -5.67 | 110.29      | 121.41   |
| 12  | A     | 468  | VAL  | O-C-N    | -5.67 | 115.48      | 122.57   |
| 10  | C     | 728  | SER  | CA-C-N   | 5.67  | 132.38      | 121.54   |
| 10  | C     | 728  | SER  | C-N-CA   | 5.67  | 132.38      | 121.54   |
| 18  | B     | 1789 | THR  | O-C-N    | -5.67 | 115.04      | 122.59   |
| 24  | D8    | 1066 | VAL  | CA-C-N   | 5.67  | 132.38      | 121.54   |
| 24  | D8    | 1066 | VAL  | C-N-CA   | 5.67  | 132.38      | 121.54   |
| 10  | C32   | 106  | GLY  | O-C-N    | -5.67 | 115.33      | 122.70   |
| 1   | R     | 304  | ASP  | CA-CB-CG | 5.67  | 118.27      | 112.60   |
| 2   | M16   | 342  | VAL  | CA-C-N   | 5.67  | 132.37      | 121.54   |
| 2   | M16   | 342  | VAL  | C-N-CA   | 5.67  | 132.37      | 121.54   |
| 18  | B8    | 1758 | GLU  | O-C-N    | 5.67  | 129.25      | 122.27   |
| 22  | I     | 129  | GLU  | CA-C-N   | 5.67  | 127.88      | 120.28   |
| 22  | I     | 129  | GLU  | C-N-CA   | 5.67  | 127.88      | 120.28   |
| 22  | I8    | 129  | GLU  | CA-C-N   | 5.67  | 127.88      | 120.28   |
| 22  | I8    | 129  | GLU  | C-N-CA   | 5.67  | 127.88      | 120.28   |
| 10  | C32   | 880  | GLU  | CA-C-N   | -5.67 | 113.50      | 121.72   |
| 10  | C32   | 880  | GLU  | C-N-CA   | -5.67 | 113.50      | 121.72   |
| 11  | A40   | 468  | VAL  | O-C-N    | -5.67 | 115.48      | 122.57   |
| 12  | A     | 124  | ASN  | O-C-N    | -5.67 | 116.11      | 122.12   |
| 10  | C8    | 1279 | THR  | O-C-N    | -5.67 | 116.86      | 123.27   |
| 24  | D32   | 1402 | ILE  | CA-C-N   | 5.67  | 132.37      | 121.54   |
| 24  | D32   | 1402 | ILE  | C-N-CA   | 5.67  | 132.37      | 121.54   |
| 5   | P8    | 442  | GLU  | O-C-N    | 5.67  | 128.61      | 122.15   |
| 10  | C24   | 1077 | ALA  | O-C-N    | -5.67 | 116.26      | 123.06   |
| 24  | D32   | 1066 | VAL  | CA-C-N   | 5.67  | 132.37      | 121.54   |
| 24  | D32   | 1066 | VAL  | C-N-CA   | 5.67  | 132.37      | 121.54   |
| 9   | K8    | 1090 | ASP  | O-C-N    | -5.67 | 116.33      | 123.01   |
| 12  | A     | 140  | TRP  | CA-C-N   | 5.67  | 128.34      | 120.29   |
| 12  | A     | 140  | TRP  | C-N-CA   | 5.67  | 128.34      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 1479 | GLY  | CA-C-N | -5.67 | 113.55      | 121.99   |
| 18  | B     | 1479 | GLY  | C-N-CA | -5.67 | 113.55      | 121.99   |
| 10  | C16   | 861  | ILE  | CA-C-N | 5.67  | 130.17      | 122.07   |
| 10  | C16   | 861  | ILE  | C-N-CA | 5.67  | 130.17      | 122.07   |
| 18  | B     | 1771 | LYS  | CA-C-N | -5.67 | 113.92      | 122.81   |
| 18  | B     | 1771 | LYS  | C-N-CA | -5.67 | 113.92      | 122.81   |
| 10  | C32   | 415  | SER  | O-C-N  | 5.67  | 128.61      | 122.15   |
| 5   | P     | 652  | LEU  | O-C-N  | 5.66  | 128.12      | 122.12   |
| 19  | 4     | 58   | GLU  | CA-C-N | -5.66 | 110.31      | 121.41   |
| 19  | 4     | 58   | GLU  | C-N-CA | -5.66 | 110.31      | 121.41   |
| 20  | E8    | 448  | LYS  | CA-C-N | 5.66  | 128.66      | 120.79   |
| 20  | E8    | 448  | LYS  | C-N-CA | 5.66  | 128.66      | 120.79   |
| 11  | A40   | 124  | ASN  | O-C-N  | -5.66 | 116.12      | 122.12   |
| 10  | C8    | 1355 | GLU  | CA-C-N | 5.66  | 132.35      | 121.54   |
| 10  | C8    | 1355 | GLU  | C-N-CA | 5.66  | 132.35      | 121.54   |
| 18  | B8    | 1479 | GLY  | CA-C-N | -5.66 | 113.56      | 121.99   |
| 18  | B8    | 1479 | GLY  | C-N-CA | -5.66 | 113.56      | 121.99   |
| 22  | I24   | 108  | LYS  | CA-C-N | 5.66  | 128.13      | 120.38   |
| 22  | I24   | 108  | LYS  | C-N-CA | 5.66  | 128.13      | 120.38   |
| 24  | D40   | 1066 | VAL  | CA-C-N | 5.66  | 132.35      | 121.54   |
| 24  | D40   | 1066 | VAL  | C-N-CA | 5.66  | 132.35      | 121.54   |
| 10  | C32   | 632  | GLN  | O-C-N  | -5.66 | 115.83      | 122.96   |
| 9   | K8    | 1239 | ASP  | O-C-N  | -5.66 | 115.46      | 122.82   |
| 10  | C24   | 632  | GLN  | O-C-N  | -5.66 | 115.83      | 122.96   |
| 24  | D     | 1066 | VAL  | CA-C-N | 5.66  | 132.35      | 121.54   |
| 24  | D     | 1066 | VAL  | C-N-CA | 5.66  | 132.35      | 121.54   |
| 10  | C32   | 1336 | ALA  | CA-C-N | 5.66  | 132.35      | 121.54   |
| 10  | C32   | 1336 | ALA  | C-N-CA | 5.66  | 132.35      | 121.54   |
| 12  | A48   | 124  | ASN  | O-C-N  | -5.66 | 116.12      | 122.12   |
| 9   | K8    | 636  | LYS  | CA-C-N | 5.66  | 130.78      | 122.63   |
| 9   | K8    | 636  | LYS  | C-N-CA | 5.66  | 130.78      | 122.63   |
| 21  | H8    | 318  | ALA  | CA-C-N | 5.66  | 132.50      | 121.41   |
| 21  | H8    | 318  | ALA  | C-N-CA | 5.66  | 132.50      | 121.41   |
| 10  | C24   | 1336 | ALA  | CA-C-N | 5.66  | 132.34      | 121.54   |
| 10  | C24   | 1336 | ALA  | C-N-CA | 5.66  | 132.34      | 121.54   |
| 22  | I16   | 108  | LYS  | CA-C-N | 5.66  | 128.13      | 120.38   |
| 22  | I16   | 108  | LYS  | C-N-CA | 5.66  | 128.13      | 120.38   |
| 18  | B     | 122  | GLU  | O-C-N  | -5.65 | 115.08      | 122.43   |
| 18  | B8    | 940  | GLY  | O-C-N  | -5.65 | 115.35      | 122.70   |
| 10  | C32   | 728  | SER  | O-C-N  | -5.65 | 115.49      | 123.01   |
| 5   | P     | 577  | SER  | O-C-N  | 5.65  | 129.22      | 122.27   |
| 10  | C16   | 289  | ASP  | CA-C-N | 5.65  | 127.86      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 289  | ASP  | C-N-CA | 5.65  | 127.86      | 120.28   |
| 18  | B8    | 122  | GLU  | O-C-N  | -5.65 | 115.08      | 122.43   |
| 10  | C16   | 1355 | GLU  | CA-C-N | 5.65  | 132.33      | 121.54   |
| 10  | C16   | 1355 | GLU  | C-N-CA | 5.65  | 132.33      | 121.54   |
| 10  | C24   | 852  | VAL  | O-C-N  | -5.65 | 116.50      | 122.83   |
| 18  | B     | 1110 | LEU  | CA-C-N | 5.65  | 131.30      | 122.26   |
| 18  | B     | 1110 | LEU  | C-N-CA | 5.65  | 131.30      | 122.26   |
| 11  | A24   | 124  | ASN  | O-C-N  | -5.65 | 116.13      | 122.12   |
| 9   | K     | 636  | LYS  | CA-C-N | 5.65  | 130.76      | 122.63   |
| 9   | K     | 636  | LYS  | C-N-CA | 5.65  | 130.76      | 122.63   |
| 9   | K     | 1029 | VAL  | O-C-N  | 5.65  | 127.57      | 121.87   |
| 18  | B8    | 1356 | SER  | O-C-N  | -5.65 | 115.61      | 122.22   |
| 20  | E     | 448  | LYS  | CA-C-N | 5.65  | 128.64      | 120.79   |
| 20  | E     | 448  | LYS  | C-N-CA | 5.65  | 128.64      | 120.79   |
| 24  | D24   | 1066 | VAL  | CA-C-N | 5.65  | 132.32      | 121.54   |
| 24  | D24   | 1066 | VAL  | C-N-CA | 5.65  | 132.32      | 121.54   |
| 10  | C32   | 289  | ASP  | CA-C-N | 5.65  | 127.85      | 120.28   |
| 10  | C32   | 289  | ASP  | C-N-CA | 5.65  | 127.85      | 120.28   |
| 10  | C8    | 1336 | ALA  | CA-C-N | 5.65  | 132.32      | 121.54   |
| 10  | C8    | 1336 | ALA  | C-N-CA | 5.65  | 132.32      | 121.54   |
| 10  | C24   | 1279 | THR  | O-C-N  | -5.64 | 116.89      | 123.27   |
| 5   | P8    | 652  | LEU  | O-C-N  | 5.64  | 128.10      | 122.12   |
| 17  | F24   | 55   | PRO  | CA-C-N | -5.64 | 115.60      | 119.66   |
| 17  | F24   | 55   | PRO  | C-N-CA | -5.64 | 115.60      | 119.66   |
| 10  | C16   | 1336 | ALA  | CA-C-N | 5.64  | 132.31      | 121.54   |
| 10  | C16   | 1336 | ALA  | C-N-CA | 5.64  | 132.31      | 121.54   |
| 24  | D40   | 1402 | ILE  | CA-C-N | 5.64  | 132.31      | 121.54   |
| 24  | D40   | 1402 | ILE  | C-N-CA | 5.64  | 132.31      | 121.54   |
| 2   | M     | 702  | VAL  | CA-C-N | 5.64  | 127.83      | 120.28   |
| 2   | M     | 702  | VAL  | C-N-CA | 5.64  | 127.83      | 120.28   |
| 10  | C24   | 415  | SER  | O-C-N  | 5.64  | 128.57      | 122.15   |
| 10  | C     | 1279 | THR  | O-C-N  | -5.64 | 116.90      | 123.27   |
| 16  | A8    | 124  | ASN  | O-C-N  | -5.64 | 116.14      | 122.12   |
| 21  | H     | 318  | ALA  | CA-C-N | 5.64  | 132.46      | 121.41   |
| 21  | H     | 318  | ALA  | C-N-CA | 5.64  | 132.46      | 121.41   |
| 2   | M     | 342  | VAL  | CA-C-N | 5.63  | 132.30      | 121.54   |
| 2   | M     | 342  | VAL  | C-N-CA | 5.63  | 132.30      | 121.54   |
| 2   | M8    | 702  | VAL  | O-C-N  | -5.63 | 116.22      | 121.97   |
| 10  | C24   | 289  | ASP  | CA-C-N | 5.63  | 127.83      | 120.28   |
| 10  | C24   | 289  | ASP  | C-N-CA | 5.63  | 127.83      | 120.28   |
| 18  | B8    | 1771 | LYS  | CA-C-N | -5.63 | 113.96      | 122.81   |
| 18  | B8    | 1771 | LYS  | C-N-CA | -5.63 | 113.96      | 122.81   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 734  | LEU  | O-C-N  | -5.63 | 115.94      | 121.18   |
| 10  | C     | 106  | GLY  | O-C-N  | -5.63 | 115.38      | 122.70   |
| 18  | B8    | 428  | GLN  | O-C-N  | -5.63 | 115.97      | 122.95   |
| 18  | B8    | 854  | SER  | CA-C-N | 5.63  | 132.45      | 121.41   |
| 18  | B8    | 854  | SER  | C-N-CA | 5.63  | 132.45      | 121.41   |
| 23  | J24   | 727  | GLY  | O-C-N  | 5.63  | 127.60      | 122.19   |
| 24  | D16   | 1402 | ILE  | CA-C-N | 5.63  | 132.30      | 121.54   |
| 24  | D16   | 1402 | ILE  | C-N-CA | 5.63  | 132.30      | 121.54   |
| 10  | C24   | 1475 | GLY  | O-C-N  | 5.63  | 127.59      | 122.18   |
| 19  | 48    | 58   | GLU  | CA-C-N | -5.63 | 110.37      | 121.41   |
| 19  | 48    | 58   | GLU  | C-N-CA | -5.63 | 110.37      | 121.41   |
| 18  | B     | 235  | ARG  | O-C-N  | 5.63  | 128.09      | 122.12   |
| 18  | B     | 688  | GLY  | CA-C-N | 5.63  | 132.29      | 121.54   |
| 18  | B     | 688  | GLY  | C-N-CA | 5.63  | 132.29      | 121.54   |
| 18  | B8    | 973  | ASP  | CA-C-N | -5.63 | 113.12      | 120.44   |
| 18  | B8    | 973  | ASP  | C-N-CA | -5.63 | 113.12      | 120.44   |
| 5   | P16   | 668  | THR  | O-C-N  | 5.63  | 128.57      | 122.15   |
| 9   | K8    | 726  | GLU  | O-C-N  | -5.63 | 115.10      | 122.59   |
| 9   | K8    | 893  | ASN  | CA-C-N | 5.63  | 132.29      | 121.54   |
| 9   | K8    | 893  | ASN  | C-N-CA | 5.63  | 132.29      | 121.54   |
| 10  | C8    | 734  | LEU  | O-C-N  | -5.63 | 115.94      | 121.18   |
| 24  | D24   | 1402 | ILE  | CA-C-N | 5.63  | 132.29      | 121.54   |
| 24  | D24   | 1402 | ILE  | C-N-CA | 5.63  | 132.29      | 121.54   |
| 10  | C16   | 515  | ASP  | CA-C-N | -5.63 | 113.13      | 120.44   |
| 10  | C16   | 515  | ASP  | C-N-CA | -5.63 | 113.13      | 120.44   |
| 10  | C32   | 861  | ILE  | CA-C-N | 5.63  | 130.12      | 122.07   |
| 10  | C32   | 861  | ILE  | C-N-CA | 5.63  | 130.12      | 122.07   |
| 10  | C16   | 147  | LEU  | O-C-N  | -5.62 | 116.76      | 123.06   |
| 11  | A24   | 468  | VAL  | O-C-N  | -5.62 | 115.54      | 122.57   |
| 10  | C24   | 1355 | GLU  | CA-C-N | 5.62  | 132.28      | 121.54   |
| 10  | C24   | 1355 | GLU  | C-N-CA | 5.62  | 132.28      | 121.54   |
| 18  | B8    | 1110 | LEU  | CA-C-N | 5.62  | 131.26      | 122.26   |
| 18  | B8    | 1110 | LEU  | C-N-CA | 5.62  | 131.26      | 122.26   |
| 21  | H24   | 318  | ALA  | CA-C-N | 5.62  | 132.43      | 121.41   |
| 21  | H24   | 318  | ALA  | C-N-CA | 5.62  | 132.43      | 121.41   |
| 10  | C8    | 252  | ASN  | CA-C-N | -5.62 | 113.06      | 122.17   |
| 10  | C8    | 252  | ASN  | C-N-CA | -5.62 | 113.06      | 122.17   |
| 18  | B8    | 688  | GLY  | CA-C-N | 5.62  | 132.28      | 121.54   |
| 18  | B8    | 688  | GLY  | C-N-CA | 5.62  | 132.28      | 121.54   |
| 10  | C32   | 1445 | THR  | CA-C-N | -5.62 | 113.60      | 122.76   |
| 10  | C32   | 1445 | THR  | C-N-CA | -5.62 | 113.60      | 122.76   |
| 9   | K8    | 1194 | GLU  | O-C-N  | 5.62  | 128.08      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | K8    | 1224 | GLY  | O-C-N   | -5.62 | 115.39      | 122.70   |
| 10  | C16   | 1445 | THR  | CA-C-N  | -5.62 | 113.60      | 122.76   |
| 10  | C16   | 1445 | THR  | C-N-CA  | -5.62 | 113.60      | 122.76   |
| 10  | C24   | 106  | GLY  | O-C-N   | -5.62 | 115.39      | 122.70   |
| 10  | C24   | 328  | HIS  | CA-C-N  | 5.62  | 128.37      | 120.28   |
| 10  | C24   | 328  | HIS  | C-N-CA  | 5.62  | 128.37      | 120.28   |
| 10  | C     | 861  | ILE  | CA-C-N  | 5.62  | 130.11      | 122.07   |
| 10  | C     | 861  | ILE  | C-N-CA  | 5.62  | 130.11      | 122.07   |
| 18  | B8    | 1789 | THR  | O-C-N   | -5.62 | 115.12      | 122.59   |
| 21  | H16   | 318  | ALA  | CA-C-N  | 5.62  | 132.42      | 121.41   |
| 21  | H16   | 318  | ALA  | C-N-CA  | 5.62  | 132.42      | 121.41   |
| 10  | C24   | 1106 | PRO  | CA-C-N  | 5.62  | 128.58      | 120.38   |
| 10  | C24   | 1106 | PRO  | C-N-CA  | 5.62  | 128.58      | 120.38   |
| 19  | 48    | 343  | LEU  | CA-C-N  | -5.62 | 114.00      | 119.78   |
| 19  | 48    | 343  | LEU  | C-N-CA  | -5.62 | 114.00      | 119.78   |
| 2   | M8    | 342  | VAL  | CA-C-N  | 5.61  | 132.26      | 121.54   |
| 2   | M8    | 342  | VAL  | C-N-CA  | 5.61  | 132.26      | 121.54   |
| 5   | P16   | 150  | PRO  | CA-C-N  | 5.61  | 128.37      | 120.28   |
| 5   | P16   | 150  | PRO  | C-N-CA  | 5.61  | 128.37      | 120.28   |
| 8   | L8    | 717  | PRO  | N-CA-CB | 5.61  | 106.33      | 103.19   |
| 9   | K     | 726  | GLU  | O-C-N   | -5.61 | 115.12      | 122.59   |
| 10  | C8    | 328  | HIS  | CA-C-N  | 5.61  | 128.36      | 120.28   |
| 10  | C8    | 328  | HIS  | C-N-CA  | 5.61  | 128.36      | 120.28   |
| 1   | R16   | 1324 | ASP  | O-C-N   | -5.61 | 114.02      | 123.00   |
| 13  | V     | 884  | ASN  | CA-C-N  | 5.61  | 132.26      | 121.54   |
| 13  | V     | 884  | ASN  | C-N-CA  | 5.61  | 132.26      | 121.54   |
| 10  | C32   | 1106 | PRO  | CA-C-N  | 5.61  | 128.57      | 120.38   |
| 10  | C32   | 1106 | PRO  | C-N-CA  | 5.61  | 128.57      | 120.38   |
| 2   | M16   | 702  | VAL  | O-C-N   | -5.61 | 116.25      | 121.97   |
| 5   | P8    | 15   | LEU  | O-C-N   | -5.61 | 115.80      | 122.20   |
| 15  | J     | 722  | LEU  | O-C-N   | -5.61 | 114.94      | 122.23   |
| 10  | C8    | 289  | ASP  | CA-C-N  | 5.61  | 127.80      | 120.28   |
| 10  | C8    | 289  | ASP  | C-N-CA  | 5.61  | 127.80      | 120.28   |
| 18  | B     | 940  | GLY  | O-C-N   | -5.61 | 115.41      | 122.70   |
| 22  | I     | 108  | LYS  | CA-C-N  | 5.61  | 128.06      | 120.38   |
| 22  | I     | 108  | LYS  | C-N-CA  | 5.61  | 128.06      | 120.38   |
| 9   | K     | 893  | ASN  | CA-C-N  | 5.61  | 132.25      | 121.54   |
| 9   | K     | 893  | ASN  | C-N-CA  | 5.61  | 132.25      | 121.54   |
| 10  | C     | 328  | HIS  | CA-C-N  | 5.61  | 128.35      | 120.28   |
| 10  | C     | 328  | HIS  | C-N-CA  | 5.61  | 128.35      | 120.28   |
| 5   | P8    | 150  | PRO  | CA-C-N  | 5.61  | 128.35      | 120.28   |
| 5   | P8    | 150  | PRO  | C-N-CA  | 5.61  | 128.35      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | B     | 1356 | SER  | O-C-N  | -5.61 | 115.66      | 122.22   |
| 20  | E     | 166  | PRO  | O-C-N  | 5.61  | 123.89      | 121.31   |
| 24  | D8    | 1402 | ILE  | CA-C-N | 5.61  | 132.25      | 121.54   |
| 24  | D8    | 1402 | ILE  | C-N-CA | 5.61  | 132.25      | 121.54   |
| 18  | B8    | 1753 | PRO  | O-C-N  | -5.60 | 116.56      | 123.01   |
| 18  | B     | 1355 | ASN  | O-C-N  | -5.60 | 115.46      | 122.35   |
| 24  | D     | 1402 | ILE  | CA-C-N | 5.60  | 132.24      | 121.54   |
| 24  | D     | 1402 | ILE  | C-N-CA | 5.60  | 132.24      | 121.54   |
| 10  | C32   | 188  | GLY  | CA-C-N | 5.60  | 126.84      | 119.84   |
| 10  | C32   | 188  | GLY  | C-N-CA | 5.60  | 126.84      | 119.84   |
| 12  | A48   | 468  | VAL  | O-C-N  | -5.60 | 115.57      | 122.57   |
| 10  | C16   | 632  | GLN  | O-C-N  | -5.60 | 115.90      | 122.96   |
| 11  | A32   | 468  | VAL  | O-C-N  | -5.60 | 115.57      | 122.57   |
| 10  | C32   | 328  | HIS  | CA-C-N | 5.60  | 128.34      | 120.28   |
| 10  | C32   | 328  | HIS  | C-N-CA | 5.60  | 128.34      | 120.28   |
| 10  | C32   | 1077 | ALA  | O-C-N  | -5.60 | 116.34      | 123.06   |
| 19  | 4     | 343  | LEU  | CA-C-N | -5.60 | 114.02      | 119.78   |
| 19  | 4     | 343  | LEU  | C-N-CA | -5.60 | 114.02      | 119.78   |
| 10  | C     | 515  | ASP  | CA-C-N | -5.60 | 113.17      | 120.44   |
| 10  | C     | 515  | ASP  | C-N-CA | -5.60 | 113.17      | 120.44   |
| 19  | 4     | 185  | GLY  | CA-C-N | -5.60 | 110.44      | 121.41   |
| 19  | 4     | 185  | GLY  | C-N-CA | -5.60 | 110.44      | 121.41   |
| 5   | P     | 150  | PRO  | CA-C-N | 5.59  | 128.34      | 120.28   |
| 5   | P     | 150  | PRO  | C-N-CA | 5.59  | 128.34      | 120.28   |
| 9   | K     | 1270 | VAL  | O-C-N  | -5.59 | 111.28      | 121.91   |
| 5   | P     | 15   | LEU  | O-C-N  | -5.59 | 115.82      | 122.20   |
| 15  | J     | 722  | LEU  | CA-C-N | 5.59  | 128.81      | 120.31   |
| 15  | J     | 722  | LEU  | C-N-CA | 5.59  | 128.81      | 120.31   |
| 18  | B8    | 607  | GLU  | CA-C-N | -5.59 | 112.23      | 120.28   |
| 18  | B8    | 607  | GLU  | C-N-CA | -5.59 | 112.23      | 120.28   |
| 9   | K     | 1194 | GLU  | O-C-N  | 5.59  | 128.04      | 122.12   |
| 10  | C16   | 1106 | PRO  | CA-C-N | 5.59  | 128.54      | 120.38   |
| 10  | C16   | 1106 | PRO  | C-N-CA | 5.59  | 128.54      | 120.38   |
| 10  | C     | 188  | GLY  | CA-C-N | 5.59  | 126.83      | 119.84   |
| 10  | C     | 188  | GLY  | C-N-CA | 5.59  | 126.83      | 119.84   |
| 19  | 48    | 185  | GLY  | CA-C-N | -5.59 | 110.45      | 121.41   |
| 19  | 48    | 185  | GLY  | C-N-CA | -5.59 | 110.45      | 121.41   |
| 10  | C32   | 1360 | GLN  | O-C-N  | 5.59  | 129.15      | 122.27   |
| 2   | M16   | 552  | PHE  | O-C-N  | -5.59 | 114.75      | 122.46   |
| 10  | C16   | 188  | GLY  | CA-C-N | 5.59  | 126.83      | 119.84   |
| 10  | C16   | 188  | GLY  | C-N-CA | 5.59  | 126.83      | 119.84   |
| 10  | C     | 852  | VAL  | O-C-N  | -5.59 | 116.57      | 122.83   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | C32   | 1475 | GLY  | O-C-N   | 5.59  | 127.54      | 122.18   |
| 10  | C8    | 515  | ASP  | CA-C-N  | -5.59 | 113.18      | 120.44   |
| 10  | C8    | 515  | ASP  | C-N-CA  | -5.59 | 113.18      | 120.44   |
| 3   | N8    | 171  | GLY  | CA-C-N  | -5.58 | 112.51      | 120.89   |
| 3   | N8    | 171  | GLY  | C-N-CA  | -5.58 | 112.51      | 120.89   |
| 10  | C16   | 252  | ASN  | CA-C-N  | -5.58 | 113.12      | 122.17   |
| 10  | C16   | 252  | ASN  | C-N-CA  | -5.58 | 113.12      | 122.17   |
| 7   | Q     | 303  | LEU  | O-C-N   | 5.58  | 127.68      | 121.43   |
| 10  | C16   | 1077 | ALA  | O-C-N   | -5.58 | 116.36      | 123.06   |
| 9   | K     | 1224 | GLY  | O-C-N   | -5.58 | 115.45      | 122.70   |
| 10  | C16   | 328  | HIS  | CA-C-N  | 5.58  | 128.31      | 120.28   |
| 10  | C16   | 328  | HIS  | C-N-CA  | 5.58  | 128.31      | 120.28   |
| 7   | Q16   | 209  | LYS  | CA-C-N  | -5.58 | 113.83      | 122.09   |
| 7   | Q16   | 209  | LYS  | C-N-CA  | -5.58 | 113.83      | 122.09   |
| 10  | C8    | 1077 | ALA  | O-C-N   | -5.58 | 116.36      | 123.06   |
| 10  | C32   | 852  | VAL  | O-C-N   | -5.58 | 116.58      | 122.83   |
| 2   | M     | 552  | PHE  | O-C-N   | -5.58 | 114.77      | 122.46   |
| 5   | P16   | 288  | ARG  | CA-C-N  | 5.58  | 124.93      | 118.85   |
| 5   | P16   | 288  | ARG  | C-N-CA  | 5.58  | 124.93      | 118.85   |
| 10  | C8    | 1331 | CYS  | CA-C-N  | 5.58  | 128.78      | 120.31   |
| 10  | C8    | 1331 | CYS  | C-N-CA  | 5.58  | 128.78      | 120.31   |
| 2   | M8    | 552  | PHE  | O-C-N   | -5.57 | 114.77      | 122.46   |
| 10  | C     | 1077 | ALA  | O-C-N   | -5.57 | 116.37      | 123.06   |
| 18  | B8    | 249  | TYR  | O-C-N   | -5.57 | 116.69      | 123.16   |
| 10  | C32   | 515  | ASP  | CA-C-N  | -5.57 | 113.19      | 120.44   |
| 10  | C32   | 515  | ASP  | C-N-CA  | -5.57 | 113.19      | 120.44   |
| 5   | P8    | 668  | THR  | O-C-N   | 5.57  | 128.50      | 122.15   |
| 8   | L     | 717  | PRO  | N-CA-CB | 5.57  | 106.31      | 103.19   |
| 3   | N     | 171  | GLY  | CA-C-N  | -5.57 | 112.53      | 120.89   |
| 3   | N     | 171  | GLY  | C-N-CA  | -5.57 | 112.53      | 120.89   |
| 3   | N16   | 171  | GLY  | CA-C-N  | -5.57 | 112.53      | 120.89   |
| 3   | N16   | 171  | GLY  | C-N-CA  | -5.57 | 112.53      | 120.89   |
| 9   | K     | 1129 | PRO  | O-C-N   | -5.57 | 115.43      | 122.17   |
| 10  | C24   | 1445 | THR  | CA-C-N  | -5.57 | 113.68      | 122.76   |
| 10  | C24   | 1445 | THR  | C-N-CA  | -5.57 | 113.68      | 122.76   |
| 10  | C32   | 916  | LEU  | CA-C-N  | 5.57  | 130.48      | 122.35   |
| 10  | C32   | 916  | LEU  | C-N-CA  | 5.57  | 130.48      | 122.35   |
| 10  | C32   | 1655 | GLN  | O-C-N   | -5.57 | 116.67      | 122.96   |
| 10  | C24   | 732  | THR  | CA-C-N  | -5.57 | 115.36      | 122.77   |
| 10  | C24   | 732  | THR  | C-N-CA  | -5.57 | 115.36      | 122.77   |
| 18  | B8    | 1048 | LYS  | O-C-N   | 5.57  | 128.50      | 122.15   |
| 7   | Q8    | 209  | LYS  | CA-C-N  | -5.57 | 113.85      | 122.09   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7   | Q8    | 209  | LYS  | C-N-CA | -5.57 | 113.85      | 122.09   |
| 9   | K8    | 1270 | VAL  | O-C-N  | -5.57 | 111.34      | 121.91   |
| 18  | B     | 435  | CYS  | O-C-N  | 5.57  | 128.02      | 122.12   |
| 10  | C24   | 1596 | GLU  | CA-C-N | 5.56  | 130.09      | 120.58   |
| 10  | C24   | 1596 | GLU  | C-N-CA | 5.56  | 130.09      | 120.58   |
| 10  | C     | 728  | SER  | O-C-N  | -5.56 | 115.61      | 123.01   |
| 5   | P     | 62   | ASP  | CA-C-N | 5.56  | 131.34      | 120.99   |
| 5   | P     | 62   | ASP  | C-N-CA | 5.56  | 131.34      | 120.99   |
| 18  | B     | 854  | SER  | CA-C-N | 5.56  | 132.31      | 121.41   |
| 18  | B     | 854  | SER  | C-N-CA | 5.56  | 132.31      | 121.41   |
| 7   | Q16   | 276  | ASN  | O-C-N  | -5.56 | 114.16      | 122.39   |
| 10  | C24   | 734  | LEU  | O-C-N  | -5.56 | 116.01      | 121.18   |
| 18  | B8    | 1355 | ASN  | O-C-N  | -5.56 | 115.51      | 122.35   |
| 1   | R     | 1148 | LYS  | O-C-N  | 5.56  | 128.49      | 122.15   |
| 1   | R     | 1324 | ASP  | O-C-N  | -5.56 | 114.11      | 123.00   |
| 5   | P     | 668  | THR  | O-C-N  | 5.56  | 128.49      | 122.15   |
| 7   | Q8    | 276  | ASN  | O-C-N  | -5.56 | 114.17      | 122.39   |
| 10  | C24   | 252  | ASN  | CA-C-N | -5.56 | 113.17      | 122.17   |
| 10  | C24   | 252  | ASN  | C-N-CA | -5.56 | 113.17      | 122.17   |
| 10  | C24   | 1331 | CYS  | CA-C-N | 5.56  | 128.76      | 120.31   |
| 10  | C24   | 1331 | CYS  | C-N-CA | 5.56  | 128.76      | 120.31   |
| 10  | C     | 1383 | GLY  | CA-C-N | 5.56  | 127.67      | 120.56   |
| 10  | C     | 1383 | GLY  | C-N-CA | 5.56  | 127.67      | 120.56   |
| 10  | C     | 734  | LEU  | O-C-N  | -5.56 | 116.01      | 121.18   |
| 20  | E8    | 426  | LEU  | O-C-N  | -5.56 | 114.98      | 122.43   |
| 3   | N     | 163  | ALA  | CA-C-N | -5.55 | 112.90      | 119.84   |
| 3   | N     | 163  | ALA  | C-N-CA | -5.55 | 112.90      | 119.84   |
| 10  | C24   | 515  | ASP  | CA-C-N | -5.55 | 113.22      | 120.44   |
| 10  | C24   | 515  | ASP  | C-N-CA | -5.55 | 113.22      | 120.44   |
| 18  | B     | 607  | GLU  | CA-C-N | -5.55 | 112.28      | 120.28   |
| 18  | B     | 607  | GLU  | C-N-CA | -5.55 | 112.28      | 120.28   |
| 10  | C32   | 734  | LEU  | O-C-N  | -5.55 | 116.01      | 121.18   |
| 7   | Q     | 276  | ASN  | O-C-N  | -5.55 | 114.17      | 122.39   |
| 18  | B     | 249  | TYR  | O-C-N  | -5.55 | 116.72      | 123.16   |
| 10  | C32   | 252  | ASN  | CA-C-N | -5.55 | 113.17      | 122.17   |
| 10  | C32   | 252  | ASN  | C-N-CA | -5.55 | 113.17      | 122.17   |
| 10  | C8    | 1445 | THR  | CA-C-N | -5.55 | 113.71      | 122.76   |
| 10  | C8    | 1445 | THR  | C-N-CA | -5.55 | 113.71      | 122.76   |
| 5   | P8    | 288  | ARG  | CA-C-N | 5.55  | 124.90      | 118.85   |
| 5   | P8    | 288  | ARG  | C-N-CA | 5.55  | 124.90      | 118.85   |
| 10  | C16   | 1383 | GLY  | CA-C-N | 5.55  | 127.66      | 120.56   |
| 10  | C16   | 1383 | GLY  | C-N-CA | 5.55  | 127.66      | 120.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | C16   | 1596 | GLU  | CA-C-N  | 5.55  | 130.07      | 120.58   |
| 10  | C16   | 1596 | GLU  | C-N-CA  | 5.55  | 130.07      | 120.58   |
| 10  | C     | 1445 | THR  | CA-C-N  | -5.55 | 113.72      | 122.76   |
| 10  | C     | 1445 | THR  | C-N-CA  | -5.55 | 113.72      | 122.76   |
| 10  | C8    | 1106 | PRO  | CA-C-N  | 5.55  | 128.48      | 120.38   |
| 10  | C8    | 1106 | PRO  | C-N-CA  | 5.55  | 128.48      | 120.38   |
| 10  | C8    | 1383 | GLY  | CA-C-N  | 5.55  | 127.66      | 120.56   |
| 10  | C8    | 1383 | GLY  | C-N-CA  | 5.55  | 127.66      | 120.56   |
| 20  | E     | 344  | PRO  | O-C-N   | -5.55 | 115.15      | 122.64   |
| 10  | C     | 1106 | PRO  | CA-C-N  | 5.55  | 128.48      | 120.38   |
| 10  | C     | 1106 | PRO  | C-N-CA  | 5.55  | 128.48      | 120.38   |
| 1   | R8    | 1324 | ASP  | O-C-N   | -5.55 | 114.13      | 123.00   |
| 10  | C24   | 861  | ILE  | CA-C-N  | 5.55  | 130.00      | 122.07   |
| 10  | C24   | 861  | ILE  | C-N-CA  | 5.55  | 130.00      | 122.07   |
| 10  | C     | 252  | ASN  | CA-C-N  | -5.55 | 113.19      | 122.17   |
| 10  | C     | 252  | ASN  | C-N-CA  | -5.55 | 113.19      | 122.17   |
| 10  | C     | 1475 | GLY  | O-C-N   | 5.55  | 127.50      | 122.18   |
| 10  | C8    | 852  | VAL  | O-C-N   | -5.55 | 116.62      | 122.83   |
| 10  | C16   | 852  | VAL  | O-C-N   | -5.54 | 116.62      | 122.83   |
| 24  | D8    | 744  | LEU  | CA-C-N  | 5.54  | 125.61      | 120.34   |
| 24  | D8    | 744  | LEU  | C-N-CA  | 5.54  | 125.61      | 120.34   |
| 1   | R16   | 1148 | LYS  | O-C-N   | 5.54  | 128.47      | 122.15   |
| 10  | C     | 1360 | GLN  | O-C-N   | 5.54  | 129.09      | 122.27   |
| 10  | C24   | 1360 | GLN  | O-C-N   | 5.54  | 129.09      | 122.27   |
| 10  | C8    | 732  | THR  | CA-C-N  | -5.54 | 115.40      | 122.77   |
| 10  | C8    | 732  | THR  | C-N-CA  | -5.54 | 115.40      | 122.77   |
| 24  | D24   | 385  | PRO  | N-CA-CB | 5.54  | 106.29      | 103.19   |
| 10  | C8    | 188  | GLY  | CA-C-N  | 5.54  | 126.76      | 119.84   |
| 10  | C8    | 188  | GLY  | C-N-CA  | 5.54  | 126.76      | 119.84   |
| 18  | B     | 1836 | LEU  | O-C-N   | 5.54  | 128.47      | 122.15   |
| 3   | N16   | 163  | ALA  | CA-C-N  | -5.54 | 112.92      | 119.84   |
| 3   | N16   | 163  | ALA  | C-N-CA  | -5.54 | 112.92      | 119.84   |
| 4   | T16   | 389  | SER  | CA-C-N  | 5.54  | 127.70      | 120.28   |
| 4   | T16   | 389  | SER  | C-N-CA  | 5.54  | 127.70      | 120.28   |
| 18  | B     | 1122 | SER  | CA-C-N  | 5.54  | 132.12      | 121.54   |
| 18  | B     | 1122 | SER  | C-N-CA  | 5.54  | 132.12      | 121.54   |
| 18  | B     | 1643 | ILE  | O-C-N   | 5.54  | 127.66      | 121.90   |
| 7   | Q     | 209  | LYS  | CA-C-N  | -5.54 | 113.90      | 122.09   |
| 7   | Q     | 209  | LYS  | C-N-CA  | -5.54 | 113.90      | 122.09   |
| 24  | D24   | 744  | LEU  | CA-C-N  | 5.53  | 125.60      | 120.34   |
| 24  | D24   | 744  | LEU  | C-N-CA  | 5.53  | 125.60      | 120.34   |
| 9   | K8    | 1129 | PRO  | O-C-N   | -5.53 | 115.48      | 122.17   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C24   | 916  | LEU  | CA-C-N | 5.53  | 130.43      | 122.35   |
| 10  | C24   | 916  | LEU  | C-N-CA | 5.53  | 130.43      | 122.35   |
| 20  | E8    | 130  | GLY  | CA-C-N | -5.53 | 112.92      | 119.84   |
| 20  | E8    | 130  | GLY  | C-N-CA | -5.53 | 112.92      | 119.84   |
| 2   | M     | 702  | VAL  | O-C-N  | -5.53 | 116.33      | 121.97   |
| 5   | P8    | 62   | ASP  | CA-C-N | 5.53  | 131.28      | 120.99   |
| 5   | P8    | 62   | ASP  | C-N-CA | 5.53  | 131.28      | 120.99   |
| 10  | C16   | 1795 | ASP  | O-C-N  | -5.53 | 116.12      | 122.09   |
| 18  | B8    | 1362 | ALA  | CA-C-N | 5.53  | 132.10      | 121.54   |
| 18  | B8    | 1362 | ALA  | C-N-CA | 5.53  | 132.10      | 121.54   |
| 18  | B     | 1048 | LYS  | O-C-N  | 5.53  | 128.45      | 122.15   |
| 20  | E     | 130  | GLY  | CA-C-N | -5.53 | 112.93      | 119.84   |
| 20  | E     | 130  | GLY  | C-N-CA | -5.53 | 112.93      | 119.84   |
| 20  | E8    | 344  | PRO  | O-C-N  | -5.53 | 115.18      | 122.64   |
| 10  | C16   | 581  | TYR  | CA-C-N | 5.53  | 128.14      | 120.29   |
| 10  | C16   | 581  | TYR  | C-N-CA | 5.53  | 128.14      | 120.29   |
| 10  | C24   | 1783 | TYR  | CA-C-N | 5.53  | 127.30      | 120.34   |
| 10  | C24   | 1783 | TYR  | C-N-CA | 5.53  | 127.30      | 120.34   |
| 10  | C32   | 581  | TYR  | CA-C-N | 5.53  | 128.14      | 120.29   |
| 10  | C32   | 581  | TYR  | C-N-CA | 5.53  | 128.14      | 120.29   |
| 10  | C32   | 1596 | GLU  | CA-C-N | 5.53  | 130.03      | 120.58   |
| 10  | C32   | 1596 | GLU  | C-N-CA | 5.53  | 130.03      | 120.58   |
| 10  | C8    | 1596 | GLU  | CA-C-N | 5.52  | 130.03      | 120.58   |
| 10  | C8    | 1596 | GLU  | C-N-CA | 5.52  | 130.03      | 120.58   |
| 5   | P8    | 679  | SER  | O-C-N  | 5.52  | 129.06      | 122.27   |
| 10  | C16   | 1475 | GLY  | O-C-N  | 5.52  | 127.48      | 122.18   |
| 10  | C8    | 581  | TYR  | CA-C-N | 5.52  | 128.13      | 120.29   |
| 10  | C8    | 581  | TYR  | C-N-CA | 5.52  | 128.13      | 120.29   |
| 10  | C8    | 1655 | GLN  | O-C-N  | -5.52 | 116.72      | 122.96   |
| 20  | E8    | 166  | PRO  | O-C-N  | 5.52  | 123.85      | 121.31   |
| 3   | N8    | 163  | ALA  | CA-C-N | -5.52 | 112.94      | 119.84   |
| 3   | N8    | 163  | ALA  | C-N-CA | -5.52 | 112.94      | 119.84   |
| 5   | P     | 679  | SER  | O-C-N  | 5.52  | 129.06      | 122.27   |
| 5   | P16   | 62   | ASP  | CA-C-N | 5.52  | 131.26      | 120.99   |
| 5   | P16   | 62   | ASP  | C-N-CA | 5.52  | 131.26      | 120.99   |
| 10  | C     | 1783 | TYR  | CA-C-N | 5.52  | 127.30      | 120.34   |
| 10  | C     | 1783 | TYR  | C-N-CA | 5.52  | 127.30      | 120.34   |
| 10  | C8    | 1805 | ASP  | O-C-N  | 5.52  | 127.97      | 122.12   |
| 18  | B8    | 1122 | SER  | CA-C-N | 5.52  | 132.08      | 121.54   |
| 18  | B8    | 1122 | SER  | C-N-CA | 5.52  | 132.08      | 121.54   |
| 20  | E     | 426  | LEU  | O-C-N  | -5.52 | 115.03      | 122.43   |
| 10  | C16   | 1045 | GLN  | O-C-N  | 5.52  | 127.97      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 1360 | GLN  | O-C-N  | 5.52  | 129.06      | 122.27   |
| 18  | B     | 1634 | LEU  | CA-C-N | 5.52  | 130.23      | 120.74   |
| 18  | B     | 1634 | LEU  | C-N-CA | 5.52  | 130.23      | 120.74   |
| 18  | B8    | 1643 | ILE  | O-C-N  | 5.52  | 127.64      | 121.90   |
| 10  | C32   | 1783 | TYR  | CA-C-N | 5.52  | 127.29      | 120.34   |
| 10  | C32   | 1783 | TYR  | C-N-CA | 5.52  | 127.29      | 120.34   |
| 2   | M     | 552  | PHE  | CA-C-N | 5.52  | 126.10      | 119.98   |
| 2   | M     | 552  | PHE  | C-N-CA | 5.52  | 126.10      | 119.98   |
| 10  | C24   | 188  | GLY  | CA-C-N | 5.52  | 126.73      | 119.84   |
| 10  | C24   | 188  | GLY  | C-N-CA | 5.52  | 126.73      | 119.84   |
| 10  | C8    | 1783 | TYR  | CA-C-N | 5.52  | 127.29      | 120.34   |
| 10  | C8    | 1783 | TYR  | C-N-CA | 5.52  | 127.29      | 120.34   |
| 5   | P     | 288  | ARG  | CA-C-N | 5.51  | 124.86      | 118.85   |
| 5   | P     | 288  | ARG  | C-N-CA | 5.51  | 124.86      | 118.85   |
| 5   | P16   | 679  | SER  | O-C-N  | 5.51  | 129.05      | 122.27   |
| 9   | K8    | 1172 | ARG  | O-C-N  | 5.51  | 128.44      | 122.15   |
| 14  | W     | 599  | ALA  | CA-C-N | 5.51  | 126.73      | 119.84   |
| 14  | W     | 599  | ALA  | C-N-CA | 5.51  | 126.73      | 119.84   |
| 18  | B     | 668  | ILE  | O-C-N  | -5.51 | 114.83      | 122.05   |
| 18  | B     | 1362 | ALA  | CA-C-N | 5.51  | 132.07      | 121.54   |
| 18  | B     | 1362 | ALA  | C-N-CA | 5.51  | 132.07      | 121.54   |
| 18  | B8    | 1189 | SER  | O-C-N  | -5.51 | 115.69      | 122.20   |
| 9   | K     | 602  | ASP  | CA-C-N | 5.51  | 131.72      | 120.80   |
| 9   | K     | 602  | ASP  | C-N-CA | 5.51  | 131.72      | 120.80   |
| 10  | C16   | 1783 | TYR  | CA-C-N | 5.51  | 127.28      | 120.34   |
| 10  | C16   | 1783 | TYR  | C-N-CA | 5.51  | 127.28      | 120.34   |
| 18  | B     | 1189 | SER  | O-C-N  | -5.51 | 115.70      | 122.20   |
| 10  | C24   | 1045 | GLN  | O-C-N  | 5.51  | 127.96      | 122.12   |
| 24  | D     | 744  | LEU  | CA-C-N | 5.51  | 125.57      | 120.34   |
| 24  | D     | 744  | LEU  | C-N-CA | 5.51  | 125.57      | 120.34   |
| 1   | R8    | 1148 | LYS  | O-C-N  | 5.51  | 128.43      | 122.15   |
| 18  | B     | 428  | GLN  | O-C-N  | -5.51 | 116.12      | 122.95   |
| 2   | M8    | 552  | PHE  | CA-C-N | 5.50  | 126.09      | 119.98   |
| 2   | M8    | 552  | PHE  | C-N-CA | 5.50  | 126.09      | 119.98   |
| 17  | F8    | 55   | PRO  | CA-C-N | -5.50 | 115.70      | 119.66   |
| 17  | F8    | 55   | PRO  | C-N-CA | -5.50 | 115.70      | 119.66   |
| 13  | V     | 885  | ARG  | CA-C-N | 5.50  | 130.36      | 122.21   |
| 13  | V     | 885  | ARG  | C-N-CA | 5.50  | 130.36      | 122.21   |
| 10  | C32   | 1383 | GLY  | CA-C-N | 5.50  | 127.60      | 120.56   |
| 10  | C32   | 1383 | GLY  | C-N-CA | 5.50  | 127.60      | 120.56   |
| 10  | C     | 601  | ASN  | O-C-N  | 5.50  | 128.42      | 122.15   |
| 10  | C8    | 1795 | ASP  | O-C-N  | -5.50 | 116.15      | 122.09   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | B     | 1753 | PRO  | O-C-N   | -5.50 | 116.68      | 123.01   |
| 24  | D40   | 385  | PRO  | N-CA-CB | 5.50  | 106.27      | 103.19   |
| 24  | D40   | 744  | LEU  | CA-C-N  | 5.50  | 125.57      | 120.34   |
| 24  | D40   | 744  | LEU  | C-N-CA  | 5.50  | 125.57      | 120.34   |
| 10  | C8    | 1360 | GLN  | O-C-N   | 5.50  | 129.04      | 122.27   |
| 10  | C16   | 991  | LEU  | O-C-N   | 5.50  | 128.42      | 122.15   |
| 2   | M     | 360  | LEU  | O-C-N   | 5.50  | 129.69      | 122.33   |
| 10  | C16   | 732  | THR  | CA-C-N  | -5.50 | 115.46      | 122.77   |
| 10  | C16   | 732  | THR  | C-N-CA  | -5.50 | 115.46      | 122.77   |
| 10  | C24   | 601  | ASN  | O-C-N   | 5.50  | 128.41      | 122.15   |
| 14  | W     | 340  | GLY  | N-CA-C  | 5.50  | 122.85      | 115.59   |
| 18  | B8    | 668  | ILE  | O-C-N   | -5.50 | 114.85      | 122.05   |
| 10  | C16   | 1655 | GLN  | O-C-N   | -5.49 | 116.75      | 122.96   |
| 10  | C     | 1596 | GLU  | CA-C-N  | 5.49  | 129.97      | 120.58   |
| 10  | C     | 1596 | GLU  | C-N-CA  | 5.49  | 129.97      | 120.58   |
| 4   | T     | 389  | SER  | CA-C-N  | 5.49  | 127.64      | 120.28   |
| 4   | T     | 389  | SER  | C-N-CA  | 5.49  | 127.64      | 120.28   |
| 10  | C32   | 601  | ASN  | O-C-N   | 5.49  | 128.41      | 122.15   |
| 10  | C16   | 1331 | CYS  | CA-C-N  | 5.49  | 128.65      | 120.31   |
| 10  | C16   | 1331 | CYS  | C-N-CA  | 5.49  | 128.65      | 120.31   |
| 10  | C     | 1655 | GLN  | O-C-N   | -5.49 | 116.75      | 122.96   |
| 17  | F16   | 55   | PRO  | CA-C-N  | -5.49 | 115.71      | 119.66   |
| 17  | F16   | 55   | PRO  | C-N-CA  | -5.49 | 115.71      | 119.66   |
| 10  | C32   | 1331 | CYS  | CA-C-N  | 5.49  | 128.66      | 120.31   |
| 10  | C32   | 1331 | CYS  | C-N-CA  | 5.49  | 128.66      | 120.31   |
| 10  | C     | 581  | TYR  | CA-C-N  | 5.49  | 128.08      | 120.29   |
| 10  | C     | 581  | TYR  | C-N-CA  | 5.49  | 128.08      | 120.29   |
| 20  | E     | 442  | LYS  | CA-C-N  | 5.49  | 132.02      | 121.54   |
| 20  | E     | 442  | LYS  | C-N-CA  | 5.49  | 132.02      | 121.54   |
| 24  | D16   | 744  | LEU  | CA-C-N  | 5.49  | 125.55      | 120.34   |
| 24  | D16   | 744  | LEU  | C-N-CA  | 5.49  | 125.55      | 120.34   |
| 18  | B8    | 1634 | LEU  | CA-C-N  | 5.49  | 130.17      | 120.74   |
| 18  | B8    | 1634 | LEU  | C-N-CA  | 5.49  | 130.17      | 120.74   |
| 9   | K8    | 602  | ASP  | CA-C-N  | 5.48  | 131.66      | 120.80   |
| 9   | K8    | 602  | ASP  | C-N-CA  | 5.48  | 131.66      | 120.80   |
| 14  | W     | 753  | THR  | CA-C-N  | -5.48 | 112.95      | 120.46   |
| 14  | W     | 753  | THR  | C-N-CA  | -5.48 | 112.95      | 120.46   |
| 10  | C     | 732  | THR  | CA-C-N  | -5.48 | 115.48      | 122.77   |
| 10  | C     | 732  | THR  | C-N-CA  | -5.48 | 115.48      | 122.77   |
| 18  | B     | 920  | ASP  | CA-C-N  | 5.48  | 128.18      | 120.28   |
| 18  | B     | 920  | ASP  | C-N-CA  | 5.48  | 128.18      | 120.28   |
| 18  | B8    | 195  | MET  | O-C-N   | -5.48 | 116.82      | 123.29   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B8    | 920  | ASP  | CA-C-N     | 5.48  | 128.18      | 120.28   |
| 18  | B8    | 920  | ASP  | C-N-CA     | 5.48  | 128.18      | 120.28   |
| 20  | E8    | 442  | LYS  | CA-C-N     | 5.48  | 132.01      | 121.54   |
| 20  | E8    | 442  | LYS  | C-N-CA     | 5.48  | 132.01      | 121.54   |
| 13  | V     | 880  | ARG  | O-C-N      | -5.48 | 115.30      | 122.59   |
| 10  | C     | 1795 | ASP  | O-C-N      | -5.48 | 116.17      | 122.09   |
| 18  | B     | 988  | SER  | O-C-N      | -5.48 | 115.30      | 122.59   |
| 18  | B8    | 988  | SER  | O-C-N      | -5.48 | 115.30      | 122.59   |
| 10  | C16   | 601  | ASN  | O-C-N      | 5.48  | 128.40      | 122.15   |
| 10  | C24   | 581  | TYR  | CA-C-N     | 5.48  | 128.07      | 120.29   |
| 10  | C24   | 581  | TYR  | C-N-CA     | 5.48  | 128.07      | 120.29   |
| 10  | C24   | 1383 | GLY  | CA-C-N     | 5.47  | 127.57      | 120.56   |
| 10  | C24   | 1383 | GLY  | C-N-CA     | 5.47  | 127.57      | 120.56   |
| 19  | 4     | 6    | HIS  | CA-C-N     | -5.47 | 113.92      | 119.83   |
| 19  | 4     | 6    | HIS  | C-N-CA     | -5.47 | 113.92      | 119.83   |
| 20  | E     | 95   | ARG  | O-C-N      | 5.47  | 127.92      | 122.12   |
| 4   | T8    | 389  | SER  | CA-C-N     | 5.47  | 127.61      | 120.28   |
| 4   | T8    | 389  | SER  | C-N-CA     | 5.47  | 127.61      | 120.28   |
| 24  | D16   | 829  | GLN  | OE1-CD-NE2 | -5.47 | 117.13      | 122.60   |
| 2   | M16   | 756  | MET  | CA-C-N     | -5.47 | 111.49      | 120.13   |
| 2   | M16   | 756  | MET  | C-N-CA     | -5.47 | 111.49      | 120.13   |
| 9   | K     | 1172 | ARG  | O-C-N      | 5.47  | 128.38      | 122.15   |
| 9   | K     | 1219 | VAL  | O-C-N      | -5.47 | 116.53      | 121.89   |
| 10  | C16   | 916  | LEU  | CA-C-N     | 5.47  | 130.33      | 122.35   |
| 10  | C16   | 916  | LEU  | C-N-CA     | 5.47  | 130.33      | 122.35   |
| 10  | C     | 1045 | GLN  | O-C-N      | 5.47  | 127.92      | 122.12   |
| 10  | C32   | 1045 | GLN  | O-C-N      | 5.47  | 127.91      | 122.12   |
| 18  | B     | 450  | CYS  | O-C-N      | 5.46  | 127.91      | 122.12   |
| 20  | E     | 224  | SER  | O-C-N      | 5.46  | 128.38      | 122.15   |
| 10  | C32   | 732  | THR  | CA-C-N     | -5.46 | 115.50      | 122.77   |
| 10  | C32   | 732  | THR  | C-N-CA     | -5.46 | 115.50      | 122.77   |
| 5   | P16   | 398  | LYS  | O-C-N      | -5.46 | 116.33      | 122.12   |
| 20  | E     | 209  | SER  | O-C-N      | -5.46 | 116.12      | 122.89   |
| 10  | C32   | 991  | LEU  | O-C-N      | 5.46  | 128.37      | 122.15   |
| 2   | M16   | 552  | PHE  | CA-C-N     | 5.46  | 126.04      | 119.98   |
| 2   | M16   | 552  | PHE  | C-N-CA     | 5.46  | 126.04      | 119.98   |
| 20  | E8    | 95   | ARG  | O-C-N      | 5.46  | 127.91      | 122.12   |
| 18  | B8    | 939  | SER  | CA-C-N     | 5.46  | 132.10      | 121.41   |
| 18  | B8    | 939  | SER  | C-N-CA     | 5.46  | 132.10      | 121.41   |
| 2   | M8    | 360  | LEU  | O-C-N      | 5.46  | 129.64      | 122.33   |
| 10  | C24   | 1805 | ASP  | O-C-N      | 5.46  | 127.90      | 122.12   |
| 18  | B8    | 1668 | PHE  | CA-C-N     | 5.46  | 126.66      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | B8    | 1668 | PHE  | C-N-CA  | 5.46  | 126.66      | 119.84   |
| 9   | K8    | 1219 | VAL  | O-C-N   | -5.45 | 116.55      | 121.89   |
| 12  | A     | 469  | VAL  | CA-C-N  | -5.45 | 111.13      | 121.54   |
| 12  | A     | 469  | VAL  | C-N-CA  | -5.45 | 111.13      | 121.54   |
| 2   | M16   | 440  | HIS  | O-C-N   | 5.45  | 128.36      | 122.15   |
| 10  | C24   | 1655 | GLN  | O-C-N   | -5.45 | 116.80      | 122.96   |
| 24  | D     | 385  | PRO  | N-CA-CB | 5.45  | 106.24      | 103.19   |
| 24  | D32   | 744  | LEU  | CA-C-N  | 5.45  | 125.52      | 120.34   |
| 24  | D32   | 744  | LEU  | C-N-CA  | 5.45  | 125.52      | 120.34   |
| 10  | C16   | 1363 | ASP  | O-C-N   | 5.45  | 127.89      | 122.12   |
| 10  | C16   | 1805 | ASP  | O-C-N   | 5.45  | 127.89      | 122.12   |
| 7   | Q16   | 261  | GLN  | O-C-N   | -5.45 | 115.35      | 122.59   |
| 10  | C     | 916  | LEU  | CA-C-N  | 5.45  | 130.30      | 122.35   |
| 10  | C     | 916  | LEU  | C-N-CA  | 5.45  | 130.30      | 122.35   |
| 18  | B8    | 161  | SER  | O-C-N   | -5.45 | 116.58      | 123.01   |
| 20  | E8    | 209  | SER  | O-C-N   | -5.45 | 116.14      | 122.89   |
| 14  | W     | 603  | LEU  | O-C-N   | -5.44 | 115.06      | 121.32   |
| 19  | 48    | 6    | HIS  | CA-C-N  | -5.44 | 113.95      | 119.83   |
| 19  | 48    | 6    | HIS  | C-N-CA  | -5.44 | 113.95      | 119.83   |
| 5   | P8    | 672  | LEU  | O-C-N   | 5.44  | 128.35      | 122.15   |
| 18  | B     | 1668 | PHE  | CA-C-N  | 5.44  | 126.64      | 119.84   |
| 18  | B     | 1668 | PHE  | C-N-CA  | 5.44  | 126.64      | 119.84   |
| 2   | M16   | 337  | ASP  | CA-C-N  | -5.44 | 112.82      | 122.07   |
| 2   | M16   | 337  | ASP  | C-N-CA  | -5.44 | 112.82      | 122.07   |
| 5   | P     | 672  | LEU  | O-C-N   | 5.44  | 128.35      | 122.15   |
| 5   | P16   | 672  | LEU  | O-C-N   | 5.44  | 128.35      | 122.15   |
| 10  | C16   | 1617 | ALA  | CA-C-N  | -5.44 | 112.36      | 121.17   |
| 10  | C16   | 1617 | ALA  | C-N-CA  | -5.44 | 112.36      | 121.17   |
| 10  | C8    | 916  | LEU  | CA-C-N  | 5.44  | 130.29      | 122.35   |
| 10  | C8    | 916  | LEU  | C-N-CA  | 5.44  | 130.29      | 122.35   |
| 24  | D24   | 1067 | SER  | N-CA-C  | 5.44  | 122.39      | 110.80   |
| 10  | C32   | 115  | ILE  | O-C-N   | 5.44  | 127.15      | 121.87   |
| 2   | M16   | 360  | LEU  | O-C-N   | 5.44  | 129.62      | 122.33   |
| 18  | B     | 709  | THR  | O-C-N   | -5.44 | 116.84      | 123.10   |
| 18  | B8    | 534  | GLY  | O-C-N   | -5.44 | 118.52      | 123.36   |
| 9   | K8    | 1241 | THR  | CA-C-N  | 5.44  | 129.91      | 121.26   |
| 9   | K8    | 1241 | THR  | C-N-CA  | 5.44  | 129.91      | 121.26   |
| 18  | B8    | 1836 | LEU  | O-C-N   | 5.44  | 128.35      | 122.15   |
| 19  | 48    | 132  | ASP  | CA-C-N  | -5.44 | 114.42      | 122.41   |
| 19  | 48    | 132  | ASP  | C-N-CA  | -5.44 | 114.42      | 122.41   |
| 9   | K     | 889  | ARG  | O-C-N   | -5.44 | 112.56      | 122.34   |
| 18  | B     | 195  | MET  | O-C-N   | -5.44 | 116.88      | 123.29   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | D8    | 385  | PRO  | N-CA-CB | 5.44  | 106.23      | 103.19   |
| 18  | B     | 939  | SER  | CA-C-N  | 5.43  | 132.06      | 121.41   |
| 18  | B     | 939  | SER  | C-N-CA  | 5.43  | 132.06      | 121.41   |
| 18  | B     | 1615 | LYS  | O-C-N   | 5.43  | 128.35      | 122.15   |
| 22  | I24   | 294  | TYR  | CA-C-N  | -5.43 | 112.86      | 122.26   |
| 22  | I24   | 294  | TYR  | C-N-CA  | -5.43 | 112.86      | 122.26   |
| 12  | A48   | 469  | VAL  | CA-C-N  | -5.43 | 111.16      | 121.54   |
| 12  | A48   | 469  | VAL  | C-N-CA  | -5.43 | 111.16      | 121.54   |
| 2   | M8    | 337  | ASP  | CA-C-N  | -5.43 | 112.83      | 122.07   |
| 2   | M8    | 337  | ASP  | C-N-CA  | -5.43 | 112.83      | 122.07   |
| 24  | D40   | 1067 | SER  | N-CA-C  | 5.43  | 122.37      | 110.80   |
| 18  | B     | 1486 | ASP  | O-C-N   | 5.43  | 127.88      | 122.12   |
| 10  | C32   | 147  | LEU  | CA-C-N  | 5.43  | 128.04      | 120.65   |
| 10  | C32   | 147  | LEU  | C-N-CA  | 5.43  | 128.04      | 120.65   |
| 1   | R     | 1138 | LEU  | CA-C-N  | 5.43  | 127.56      | 120.28   |
| 1   | R     | 1138 | LEU  | C-N-CA  | 5.43  | 127.56      | 120.28   |
| 3   | N16   | 231  | SER  | CA-C-N  | 5.43  | 128.07      | 122.80   |
| 3   | N16   | 231  | SER  | C-N-CA  | 5.43  | 128.07      | 122.80   |
| 9   | K     | 1241 | THR  | CA-C-N  | 5.43  | 129.89      | 121.26   |
| 9   | K     | 1241 | THR  | C-N-CA  | 5.43  | 129.89      | 121.26   |
| 14  | W     | 605  | ASN  | O-C-N   | 5.43  | 128.95      | 122.27   |
| 10  | C     | 428  | GLY  | CA-C-N  | 5.43  | 129.68      | 120.88   |
| 10  | C     | 428  | GLY  | C-N-CA  | 5.43  | 129.68      | 120.88   |
| 9   | K8    | 1098 | LYS  | O-C-N   | 5.43  | 128.57      | 122.22   |
| 20  | E8    | 224  | SER  | O-C-N   | 5.42  | 128.33      | 122.15   |
| 1   | R16   | 1138 | LEU  | CA-C-N  | 5.42  | 127.54      | 120.28   |
| 1   | R16   | 1138 | LEU  | C-N-CA  | 5.42  | 127.54      | 120.28   |
| 7   | Q     | 65   | ASN  | O-C-N   | 5.42  | 126.13      | 121.30   |
| 7   | Q     | 261  | GLN  | O-C-N   | -5.42 | 115.38      | 122.59   |
| 18  | B8    | 1230 | GLY  | CA-C-N  | 5.42  | 131.07      | 120.99   |
| 18  | B8    | 1230 | GLY  | C-N-CA  | 5.42  | 131.07      | 120.99   |
| 10  | C32   | 1617 | ALA  | CA-C-N  | -5.42 | 112.39      | 121.17   |
| 10  | C32   | 1617 | ALA  | C-N-CA  | -5.42 | 112.39      | 121.17   |
| 10  | C24   | 1617 | ALA  | CA-C-N  | -5.42 | 112.39      | 121.17   |
| 10  | C24   | 1617 | ALA  | C-N-CA  | -5.42 | 112.39      | 121.17   |
| 9   | K8    | 889  | ARG  | O-C-N   | -5.42 | 112.59      | 122.34   |
| 2   | M     | 337  | ASP  | CA-C-N  | -5.42 | 112.86      | 122.07   |
| 2   | M     | 337  | ASP  | C-N-CA  | -5.42 | 112.86      | 122.07   |
| 10  | C16   | 428  | GLY  | CA-C-N  | 5.42  | 129.65      | 120.88   |
| 10  | C16   | 428  | GLY  | C-N-CA  | 5.42  | 129.65      | 120.88   |
| 10  | C24   | 115  | ILE  | O-C-N   | 5.42  | 127.12      | 121.87   |
| 13  | V     | 880  | ARG  | CA-C-N  | -5.42 | 110.80      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 13  | V     | 880  | ARG  | C-N-CA     | -5.42 | 110.80      | 121.41   |
| 24  | D32   | 385  | PRO  | N-CA-CB    | 5.41  | 106.22      | 103.19   |
| 10  | C32   | 1805 | ASP  | O-C-N      | 5.41  | 127.86      | 122.12   |
| 10  | C24   | 533  | ALA  | O-C-N      | -5.41 | 116.91      | 123.13   |
| 22  | I     | 294  | TYR  | CA-C-N     | -5.41 | 112.90      | 122.26   |
| 22  | I     | 294  | TYR  | C-N-CA     | -5.41 | 112.90      | 122.26   |
| 2   | M8    | 440  | HIS  | O-C-N      | 5.41  | 128.32      | 122.15   |
| 10  | C16   | 533  | ALA  | O-C-N      | -5.41 | 116.91      | 123.13   |
| 11  | A24   | 469  | VAL  | CA-C-N     | -5.41 | 111.21      | 121.54   |
| 11  | A24   | 469  | VAL  | C-N-CA     | -5.41 | 111.21      | 121.54   |
| 19  | 4     | 132  | ASP  | CA-C-N     | -5.41 | 114.46      | 122.41   |
| 19  | 4     | 132  | ASP  | C-N-CA     | -5.41 | 114.46      | 122.41   |
| 24  | D     | 1067 | SER  | N-CA-C     | 5.41  | 122.33      | 110.80   |
| 10  | C24   | 152  | ILE  | O-C-N      | 5.41  | 127.12      | 121.87   |
| 10  | C8    | 601  | ASN  | O-C-N      | 5.41  | 128.32      | 122.15   |
| 18  | B     | 1230 | GLY  | CA-C-N     | 5.41  | 131.05      | 120.99   |
| 18  | B     | 1230 | GLY  | C-N-CA     | 5.41  | 131.05      | 120.99   |
| 24  | D8    | 1067 | SER  | N-CA-C     | 5.41  | 122.32      | 110.80   |
| 2   | M8    | 756  | MET  | CA-C-N     | -5.41 | 111.59      | 120.13   |
| 2   | M8    | 756  | MET  | C-N-CA     | -5.41 | 111.59      | 120.13   |
| 7   | Q8    | 261  | GLN  | O-C-N      | -5.41 | 115.40      | 122.59   |
| 23  | J8    | 723  | GLN  | O-C-N      | -5.41 | 115.19      | 122.43   |
| 3   | N     | 231  | SER  | CA-C-N     | 5.41  | 128.04      | 122.80   |
| 3   | N     | 231  | SER  | C-N-CA     | 5.41  | 128.04      | 122.80   |
| 14  | W     | 206  | GLN  | OE1-CD-NE2 | -5.41 | 117.19      | 122.60   |
| 10  | C24   | 428  | GLY  | CA-C-N     | 5.40  | 129.63      | 120.88   |
| 10  | C24   | 428  | GLY  | C-N-CA     | 5.40  | 129.63      | 120.88   |
| 10  | C     | 1805 | ASP  | O-C-N      | 5.40  | 127.85      | 122.12   |
| 11  | A32   | 639  | GLY  | O-C-N      | 5.40  | 127.36      | 122.88   |
| 5   | P8    | 398  | LYS  | O-C-N      | -5.40 | 116.39      | 122.12   |
| 13  | V     | 895  | LEU  | O-C-N      | 5.40  | 128.91      | 122.27   |
| 10  | C8    | 1045 | GLN  | O-C-N      | 5.40  | 127.84      | 122.12   |
| 11  | A32   | 99   | THR  | O-C-N      | -5.40 | 115.34      | 122.42   |
| 11  | A24   | 38   | ASP  | O-C-N      | 5.40  | 127.84      | 122.12   |
| 10  | C24   | 653  | TYR  | O-C-N      | -5.40 | 115.11      | 121.32   |
| 22  | I8    | 294  | TYR  | CA-C-N     | -5.40 | 112.92      | 122.26   |
| 22  | I8    | 294  | TYR  | C-N-CA     | -5.40 | 112.92      | 122.26   |
| 24  | D16   | 1067 | SER  | N-CA-C     | 5.40  | 122.29      | 110.80   |
| 24  | D32   | 1067 | SER  | N-CA-C     | 5.40  | 122.29      | 110.80   |
| 3   | N8    | 231  | SER  | CA-C-N     | 5.39  | 128.03      | 122.80   |
| 3   | N8    | 231  | SER  | C-N-CA     | 5.39  | 128.03      | 122.80   |
| 11  | A40   | 38   | ASP  | O-C-N      | 5.39  | 127.84      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 13  | V     | 831  | LYS  | O-C-N      | -5.39 | 116.88      | 123.30   |
| 18  | B8    | 709  | THR  | O-C-N      | -5.39 | 116.90      | 123.10   |
| 10  | C     | 1617 | ALA  | CA-C-N     | -5.39 | 112.43      | 121.17   |
| 10  | C     | 1617 | ALA  | C-N-CA     | -5.39 | 112.43      | 121.17   |
| 11  | A16   | 99   | THR  | O-C-N      | -5.39 | 115.36      | 122.42   |
| 18  | B8    | 1013 | VAL  | O-C-N      | -5.39 | 116.42      | 121.87   |
| 24  | D16   | 385  | PRO  | N-CA-CB    | 5.39  | 106.21      | 103.19   |
| 2   | M     | 244  | PHE  | O-C-N      | -5.39 | 115.64      | 121.95   |
| 18  | B8    | 1617 | GLN  | O-C-N      | 5.39  | 128.30      | 122.15   |
| 10  | C32   | 1363 | ASP  | O-C-N      | 5.39  | 127.83      | 122.12   |
| 2   | M16   | 404  | ASP  | O-C-N      | 5.39  | 128.29      | 122.15   |
| 5   | P     | 398  | LYS  | O-C-N      | -5.39 | 116.41      | 122.12   |
| 10  | C16   | 115  | ILE  | O-C-N      | 5.39  | 127.10      | 121.87   |
| 14  | W     | 777  | LEU  | O-C-N      | 5.39  | 128.29      | 122.15   |
| 10  | C     | 1386 | ASP  | O-C-N      | 5.39  | 127.83      | 122.12   |
| 10  | C8    | 152  | ILE  | O-C-N      | 5.39  | 127.10      | 121.87   |
| 11  | A32   | 469  | VAL  | CA-C-N     | -5.39 | 111.25      | 121.54   |
| 11  | A32   | 469  | VAL  | C-N-CA     | -5.39 | 111.25      | 121.54   |
| 22  | I16   | 294  | TYR  | CA-C-N     | -5.39 | 112.94      | 122.26   |
| 22  | I16   | 294  | TYR  | C-N-CA     | -5.39 | 112.94      | 122.26   |
| 17  | F     | 55   | PRO  | CA-C-N     | -5.39 | 115.78      | 119.66   |
| 17  | F     | 55   | PRO  | C-N-CA     | -5.39 | 115.78      | 119.66   |
| 23  | J24   | 723  | GLN  | O-C-N      | -5.39 | 115.21      | 122.43   |
| 1   | R8    | 1138 | LEU  | CA-C-N     | 5.39  | 127.50      | 120.28   |
| 1   | R8    | 1138 | LEU  | C-N-CA     | 5.39  | 127.50      | 120.28   |
| 18  | B     | 534  | GLY  | O-C-N      | -5.39 | 118.57      | 123.36   |
| 18  | B     | 1264 | GLN  | O-C-N      | 5.39  | 127.83      | 122.12   |
| 10  | C24   | 580  | GLY  | CA-C-N     | -5.38 | 114.60      | 122.19   |
| 10  | C24   | 580  | GLY  | C-N-CA     | -5.38 | 114.60      | 122.19   |
| 24  | D24   | 829  | GLN  | OE1-CD-NE2 | -5.38 | 117.22      | 122.60   |
| 10  | C24   | 147  | LEU  | CA-C-N     | 5.38  | 127.97      | 120.65   |
| 10  | C24   | 147  | LEU  | C-N-CA     | 5.38  | 127.97      | 120.65   |
| 3   | N     | 160  | PRO  | CA-C-N     | 5.38  | 128.49      | 120.31   |
| 3   | N     | 160  | PRO  | C-N-CA     | 5.38  | 128.49      | 120.31   |
| 5   | P8    | 150  | PRO  | O-C-N      | -5.38 | 116.28      | 122.85   |
| 10  | C16   | 1491 | CYS  | O-C-N      | -5.38 | 115.51      | 122.77   |
| 10  | C     | 427  | ASP  | O-C-N      | -5.38 | 114.76      | 122.29   |
| 10  | C24   | 1177 | ARG  | O-C-N      | 5.38  | 127.82      | 122.12   |
| 10  | C     | 533  | ALA  | O-C-N      | -5.38 | 116.94      | 123.13   |
| 10  | C32   | 653  | TYR  | CA-C-N     | 5.38  | 125.02      | 119.05   |
| 10  | C32   | 653  | TYR  | C-N-CA     | 5.38  | 125.02      | 119.05   |
| 2   | M8    | 404  | ASP  | O-C-N      | 5.38  | 128.28      | 122.15   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10  | C     | 152  | ILE  | O-C-N    | 5.38  | 127.09      | 121.87   |
| 10  | C     | 1363 | ASP  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 10  | C8    | 1617 | ALA  | CA-C-N   | -5.38 | 112.46      | 121.17   |
| 10  | C8    | 1617 | ALA  | C-N-CA   | -5.38 | 112.46      | 121.17   |
| 18  | B8    | 770  | LEU  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 9   | K     | 733  | LEU  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 10  | C     | 1177 | ARG  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 10  | C8    | 991  | LEU  | O-C-N    | 5.38  | 128.28      | 122.15   |
| 11  | A32   | 38   | ASP  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 18  | B8    | 450  | CYS  | O-C-N    | 5.38  | 127.82      | 122.12   |
| 9   | K8    | 733  | LEU  | O-C-N    | 5.37  | 127.82      | 122.12   |
| 10  | C16   | 427  | ASP  | O-C-N    | -5.37 | 114.77      | 122.29   |
| 10  | C24   | 653  | TYR  | CA-C-N   | 5.37  | 125.02      | 119.05   |
| 10  | C24   | 653  | TYR  | C-N-CA   | 5.37  | 125.02      | 119.05   |
| 10  | C     | 1340 | PRO  | CA-C-N   | 5.37  | 128.22      | 120.38   |
| 10  | C     | 1340 | PRO  | C-N-CA   | 5.37  | 128.22      | 120.38   |
| 11  | A24   | 462  | THR  | CA-C-N   | 5.37  | 131.94      | 121.41   |
| 11  | A24   | 462  | THR  | C-N-CA   | 5.37  | 131.94      | 121.41   |
| 10  | C24   | 1806 | ARG  | CA-C-N   | 5.37  | 128.01      | 120.28   |
| 10  | C24   | 1806 | ARG  | C-N-CA   | 5.37  | 128.01      | 120.28   |
| 11  | A40   | 469  | VAL  | CA-C-N   | -5.37 | 111.28      | 121.54   |
| 11  | A40   | 469  | VAL  | C-N-CA   | -5.37 | 111.28      | 121.54   |
| 11  | A16   | 462  | THR  | CA-C-N   | 5.37  | 131.94      | 121.41   |
| 11  | A16   | 462  | THR  | C-N-CA   | 5.37  | 131.94      | 121.41   |
| 11  | A16   | 639  | GLY  | O-C-N    | 5.37  | 127.34      | 122.88   |
| 12  | A48   | 834  | ARG  | O-C-N    | 5.37  | 127.81      | 122.12   |
| 2   | M8    | 244  | PHE  | O-C-N    | -5.37 | 115.67      | 121.95   |
| 3   | N8    | 160  | PRO  | CA-C-N   | 5.37  | 128.47      | 120.31   |
| 3   | N8    | 160  | PRO  | C-N-CA   | 5.37  | 128.47      | 120.31   |
| 10  | C16   | 580  | GLY  | CA-C-N   | -5.37 | 114.62      | 122.19   |
| 10  | C16   | 580  | GLY  | C-N-CA   | -5.37 | 114.62      | 122.19   |
| 18  | B8    | 1615 | LYS  | O-C-N    | 5.37  | 128.27      | 122.15   |
| 18  | B8    | 1905 | MET  | O-C-N    | 5.37  | 127.81      | 122.12   |
| 10  | C32   | 1491 | CYS  | O-C-N    | -5.37 | 115.52      | 122.77   |
| 4   | T     | 328  | ASP  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 10  | C16   | 653  | TYR  | CA-C-N   | 5.37  | 125.01      | 119.05   |
| 10  | C16   | 653  | TYR  | C-N-CA   | 5.37  | 125.01      | 119.05   |
| 10  | C32   | 428  | GLY  | CA-C-N   | 5.37  | 129.57      | 120.88   |
| 10  | C32   | 428  | GLY  | C-N-CA   | 5.37  | 129.57      | 120.88   |
| 10  | C8    | 1363 | ASP  | O-C-N    | 5.37  | 127.81      | 122.12   |
| 10  | C32   | 580  | GLY  | CA-C-N   | -5.37 | 114.62      | 122.19   |
| 10  | C32   | 580  | GLY  | C-N-CA   | -5.37 | 114.62      | 122.19   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | M     | 756  | MET  | CA-C-N   | -5.36 | 111.66      | 120.13   |
| 2   | M     | 756  | MET  | C-N-CA   | -5.36 | 111.66      | 120.13   |
| 7   | Q8    | 65   | ASN  | O-C-N    | 5.36  | 126.07      | 121.30   |
| 10  | C     | 115  | ILE  | O-C-N    | 5.36  | 127.07      | 121.87   |
| 11  | A32   | 462  | THR  | CA-C-N   | 5.36  | 131.92      | 121.41   |
| 11  | A32   | 462  | THR  | C-N-CA   | 5.36  | 131.92      | 121.41   |
| 12  | A     | 449  | ASP  | O-C-N    | 5.36  | 127.80      | 122.12   |
| 14  | W     | 788  | ASN  | O-C-N    | 5.36  | 127.80      | 122.12   |
| 10  | C8    | 428  | GLY  | CA-C-N   | 5.36  | 129.57      | 120.88   |
| 10  | C8    | 428  | GLY  | C-N-CA   | 5.36  | 129.57      | 120.88   |
| 10  | C8    | 580  | GLY  | CA-C-N   | -5.36 | 114.63      | 122.19   |
| 10  | C8    | 580  | GLY  | C-N-CA   | -5.36 | 114.63      | 122.19   |
| 10  | C     | 653  | TYR  | CA-C-N   | 5.36  | 125.00      | 119.05   |
| 10  | C     | 653  | TYR  | C-N-CA   | 5.36  | 125.00      | 119.05   |
| 15  | J     | 681  | GLU  | O-C-N    | -5.36 | 116.44      | 122.12   |
| 3   | N16   | 160  | PRO  | CA-C-N   | 5.36  | 128.45      | 120.31   |
| 3   | N16   | 160  | PRO  | C-N-CA   | 5.36  | 128.45      | 120.31   |
| 10  | C16   | 147  | LEU  | CA-C-N   | 5.36  | 127.94      | 120.65   |
| 10  | C16   | 147  | LEU  | C-N-CA   | 5.36  | 127.94      | 120.65   |
| 10  | C     | 1491 | CYS  | O-C-N    | -5.36 | 115.54      | 122.77   |
| 18  | B8    | 124  | THR  | CA-C-N   | 5.36  | 131.77      | 121.54   |
| 18  | B8    | 124  | THR  | C-N-CA   | 5.36  | 131.77      | 121.54   |
| 4   | T16   | 328  | ASP  | CA-CB-CG | 5.36  | 117.95      | 112.60   |
| 9   | K     | 1098 | LYS  | O-C-N    | 5.36  | 128.49      | 122.22   |
| 11  | A40   | 639  | GLY  | O-C-N    | 5.36  | 127.33      | 122.88   |
| 10  | C8    | 147  | LEU  | CA-C-N   | 5.36  | 127.93      | 120.65   |
| 10  | C8    | 147  | LEU  | C-N-CA   | 5.36  | 127.93      | 120.65   |
| 10  | C8    | 861  | ILE  | O-C-N    | -5.36 | 115.88      | 122.57   |
| 11  | A32   | 834  | ARG  | O-C-N    | 5.36  | 127.80      | 122.12   |
| 10  | C32   | 427  | ASP  | O-C-N    | -5.36 | 114.79      | 122.29   |
| 10  | C     | 43   | LEU  | CA-C-N   | 5.35  | 131.46      | 123.05   |
| 10  | C     | 43   | LEU  | C-N-CA   | 5.35  | 131.46      | 123.05   |
| 10  | C8    | 43   | LEU  | CA-C-N   | 5.35  | 131.46      | 123.05   |
| 10  | C8    | 43   | LEU  | C-N-CA   | 5.35  | 131.46      | 123.05   |
| 24  | D8    | 745  | GLY  | CA-C-N   | 5.35  | 131.77      | 121.54   |
| 24  | D8    | 745  | GLY  | C-N-CA   | 5.35  | 131.77      | 121.54   |
| 12  | A48   | 157  | LEU  | O-C-N    | 5.35  | 126.02      | 121.20   |
| 2   | M     | 701  | SER  | O-C-N    | -5.35 | 116.26      | 121.93   |
| 11  | A40   | 462  | THR  | CA-C-N   | 5.35  | 131.90      | 121.41   |
| 11  | A40   | 462  | THR  | C-N-CA   | 5.35  | 131.90      | 121.41   |
| 10  | C     | 147  | LEU  | CA-C-N   | 5.35  | 127.93      | 120.65   |
| 10  | C     | 147  | LEU  | C-N-CA   | 5.35  | 127.93      | 120.65   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10  | C     | 667  | ILE  | O-C-N      | 5.35  | 127.85      | 121.80   |
| 10  | C8    | 1386 | ASP  | O-C-N      | 5.35  | 127.79      | 122.12   |
| 18  | B     | 1617 | GLN  | O-C-N      | 5.35  | 128.25      | 122.15   |
| 18  | B8    | 958  | ARG  | CA-C-N     | -5.35 | 113.83      | 122.24   |
| 18  | B8    | 958  | ARG  | C-N-CA     | -5.35 | 113.83      | 122.24   |
| 18  | B8    | 1105 | LEU  | O-C-N      | 5.35  | 128.25      | 122.15   |
| 10  | C32   | 533  | ALA  | O-C-N      | -5.35 | 116.97      | 123.13   |
| 10  | C     | 991  | LEU  | O-C-N      | 5.35  | 128.25      | 122.15   |
| 18  | B     | 161  | SER  | O-C-N      | -5.35 | 116.70      | 123.01   |
| 24  | D     | 829  | GLN  | OE1-CD-NE2 | -5.35 | 117.25      | 122.60   |
| 10  | C32   | 682  | SER  | CA-C-N     | 5.35  | 130.55      | 122.42   |
| 10  | C32   | 682  | SER  | C-N-CA     | 5.35  | 130.55      | 122.42   |
| 10  | C8    | 427  | ASP  | O-C-N      | -5.35 | 114.80      | 122.29   |
| 3   | N     | 66   | HIS  | CA-C-N     | 5.35  | 125.02      | 119.56   |
| 3   | N     | 66   | HIS  | C-N-CA     | 5.35  | 125.02      | 119.56   |
| 5   | P16   | 150  | PRO  | O-C-N      | -5.35 | 116.33      | 122.85   |
| 11  | A24   | 157  | LEU  | O-C-N      | 5.35  | 126.01      | 121.20   |
| 18  | B     | 1924 | GLY  | CA-C-N     | 5.35  | 129.72      | 120.58   |
| 18  | B     | 1924 | GLY  | C-N-CA     | 5.35  | 129.72      | 120.58   |
| 12  | A48   | 462  | THR  | CA-C-N     | 5.35  | 131.89      | 121.41   |
| 12  | A48   | 462  | THR  | C-N-CA     | 5.35  | 131.89      | 121.41   |
| 2   | M16   | 701  | SER  | O-C-N      | -5.34 | 116.27      | 121.93   |
| 10  | C24   | 847  | ARG  | CA-C-N     | 5.34  | 129.15      | 120.60   |
| 10  | C24   | 847  | ARG  | C-N-CA     | 5.34  | 129.15      | 120.60   |
| 10  | C8    | 1177 | ARG  | O-C-N      | 5.34  | 127.78      | 122.12   |
| 18  | B     | 958  | ARG  | CA-C-N     | -5.34 | 113.85      | 122.24   |
| 18  | B     | 958  | ARG  | C-N-CA     | -5.34 | 113.85      | 122.24   |
| 18  | B8    | 1924 | GLY  | CA-C-N     | 5.34  | 129.72      | 120.58   |
| 18  | B8    | 1924 | GLY  | C-N-CA     | 5.34  | 129.72      | 120.58   |
| 24  | D40   | 829  | GLN  | OE1-CD-NE2 | -5.34 | 117.26      | 122.60   |
| 2   | M     | 404  | ASP  | O-C-N      | 5.34  | 128.24      | 122.15   |
| 4   | T8    | 328  | ASP  | CA-CB-CG   | 5.34  | 117.94      | 112.60   |
| 9   | K     | 1155 | THR  | O-C-N      | -5.34 | 116.43      | 122.68   |
| 10  | C     | 847  | ARG  | CA-C-N     | 5.34  | 129.15      | 120.60   |
| 10  | C     | 847  | ARG  | C-N-CA     | 5.34  | 129.15      | 120.60   |
| 10  | C8    | 1491 | CYS  | O-C-N      | -5.34 | 115.56      | 122.77   |
| 11  | A16   | 469  | VAL  | CA-C-N     | -5.34 | 111.34      | 121.54   |
| 11  | A16   | 469  | VAL  | C-N-CA     | -5.34 | 111.34      | 121.54   |
| 18  | B     | 124  | THR  | CA-C-N     | 5.34  | 131.74      | 121.54   |
| 18  | B     | 124  | THR  | C-N-CA     | 5.34  | 131.74      | 121.54   |
| 19  | 48    | 372  | LYS  | CA-C-N     | -5.34 | 113.22      | 121.45   |
| 19  | 48    | 372  | LYS  | C-N-CA     | -5.34 | 113.22      | 121.45   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23  | J8    | 684  | ASP  | O-C-N      | -5.34 | 115.41      | 122.57   |
| 10  | C     | 580  | GLY  | CA-C-N     | -5.34 | 114.66      | 122.19   |
| 10  | C     | 580  | GLY  | C-N-CA     | -5.34 | 114.66      | 122.19   |
| 10  | C     | 653  | TYR  | O-C-N      | -5.34 | 115.18      | 121.32   |
| 10  | C8    | 1771 | GLN  | CA-C-N     | 5.34  | 130.82      | 122.17   |
| 10  | C8    | 1771 | GLN  | C-N-CA     | 5.34  | 130.82      | 122.17   |
| 18  | B     | 1105 | LEU  | O-C-N      | 5.34  | 128.24      | 122.15   |
| 10  | C32   | 1340 | PRO  | CA-C-N     | 5.34  | 128.17      | 120.38   |
| 10  | C32   | 1340 | PRO  | C-N-CA     | 5.34  | 128.17      | 120.38   |
| 11  | A16   | 449  | ASP  | O-C-N      | 5.34  | 127.78      | 122.12   |
| 10  | C24   | 427  | ASP  | O-C-N      | -5.33 | 114.82      | 122.29   |
| 10  | C8    | 1806 | ARG  | CA-C-N     | 5.33  | 127.96      | 120.28   |
| 10  | C8    | 1806 | ARG  | C-N-CA     | 5.33  | 127.96      | 120.28   |
| 23  | J24   | 684  | ASP  | O-C-N      | -5.33 | 115.42      | 122.57   |
| 24  | D     | 745  | GLY  | CA-C-N     | 5.33  | 131.73      | 121.54   |
| 24  | D     | 745  | GLY  | C-N-CA     | 5.33  | 131.73      | 121.54   |
| 24  | D8    | 829  | GLN  | OE1-CD-NE2 | -5.33 | 117.27      | 122.60   |
| 24  | D24   | 745  | GLY  | CA-C-N     | 5.33  | 131.73      | 121.54   |
| 24  | D24   | 745  | GLY  | C-N-CA     | 5.33  | 131.73      | 121.54   |
| 2   | M     | 326  | GLN  | O-C-N      | -5.33 | 115.50      | 122.59   |
| 2   | M     | 440  | HIS  | O-C-N      | 5.33  | 128.23      | 122.15   |
| 2   | M8    | 701  | SER  | O-C-N      | -5.33 | 116.28      | 121.93   |
| 5   | P     | 150  | PRO  | O-C-N      | -5.33 | 116.34      | 122.85   |
| 10  | C8    | 653  | TYR  | CA-C-N     | 5.33  | 124.97      | 119.05   |
| 10  | C8    | 653  | TYR  | C-N-CA     | 5.33  | 124.97      | 119.05   |
| 18  | B8    | 202  | LEU  | O-C-N      | 5.33  | 127.77      | 122.12   |
| 19  | 4     | 282  | GLU  | O-C-N      | -5.33 | 117.14      | 123.22   |
| 5   | P     | 207  | HIS  | CA-C-N     | -5.33 | 114.27      | 119.76   |
| 5   | P     | 207  | HIS  | C-N-CA     | -5.33 | 114.27      | 119.76   |
| 10  | C16   | 847  | ARG  | CA-C-N     | 5.33  | 129.13      | 120.60   |
| 10  | C16   | 847  | ARG  | C-N-CA     | 5.33  | 129.13      | 120.60   |
| 18  | B     | 1905 | MET  | O-C-N      | 5.33  | 127.77      | 122.12   |
| 10  | C32   | 653  | TYR  | O-C-N      | -5.33 | 115.19      | 121.32   |
| 10  | C16   | 1806 | ARG  | CA-C-N     | 5.33  | 127.96      | 120.28   |
| 10  | C16   | 1806 | ARG  | C-N-CA     | 5.33  | 127.96      | 120.28   |
| 10  | C24   | 43   | LEU  | CA-C-N     | 5.33  | 131.42      | 123.05   |
| 10  | C24   | 43   | LEU  | C-N-CA     | 5.33  | 131.42      | 123.05   |
| 13  | V     | 827  | TRP  | CA-C-N     | 5.33  | 127.86      | 120.29   |
| 13  | V     | 827  | TRP  | C-N-CA     | 5.33  | 127.86      | 120.29   |
| 3   | N8    | 66   | HIS  | CA-C-N     | 5.33  | 124.99      | 119.56   |
| 3   | N8    | 66   | HIS  | C-N-CA     | 5.33  | 124.99      | 119.56   |
| 18  | B     | 770  | LEU  | O-C-N      | 5.33  | 127.77      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23  | J16   | 684  | ASP  | O-C-N      | -5.33 | 115.43      | 122.57   |
| 24  | D16   | 745  | GLY  | CA-C-N     | 5.33  | 131.72      | 121.54   |
| 24  | D16   | 745  | GLY  | C-N-CA     | 5.33  | 131.72      | 121.54   |
| 24  | D24   | 681  | ASP  | CA-C-N     | 5.33  | 131.72      | 121.54   |
| 24  | D24   | 681  | ASP  | C-N-CA     | 5.33  | 131.72      | 121.54   |
| 10  | C32   | 43   | LEU  | CA-C-N     | 5.33  | 131.42      | 123.05   |
| 10  | C32   | 43   | LEU  | C-N-CA     | 5.33  | 131.42      | 123.05   |
| 18  | B8    | 1486 | ASP  | O-C-N      | 5.33  | 127.77      | 122.12   |
| 24  | D32   | 829  | GLN  | OE1-CD-NE2 | -5.33 | 117.27      | 122.60   |
| 24  | D40   | 745  | GLY  | CA-C-N     | 5.33  | 131.72      | 121.54   |
| 24  | D40   | 745  | GLY  | C-N-CA     | 5.33  | 131.72      | 121.54   |
| 10  | C16   | 1386 | ASP  | O-C-N      | 5.33  | 127.77      | 122.12   |
| 10  | C24   | 1340 | PRO  | CA-C-N     | 5.33  | 128.16      | 120.38   |
| 10  | C24   | 1340 | PRO  | C-N-CA     | 5.33  | 128.16      | 120.38   |
| 14  | W     | 708  | PRO  | CA-C-N     | 5.33  | 128.33      | 120.82   |
| 14  | W     | 708  | PRO  | C-N-CA     | 5.33  | 128.33      | 120.82   |
| 18  | B8    | 485  | ASN  | O-C-N      | 5.32  | 127.76      | 122.12   |
| 23  | J16   | 723  | GLN  | O-C-N      | -5.32 | 115.30      | 122.43   |
| 24  | D32   | 681  | ASP  | CA-C-N     | 5.32  | 131.71      | 121.54   |
| 24  | D32   | 681  | ASP  | C-N-CA     | 5.32  | 131.71      | 121.54   |
| 10  | C32   | 1538 | THR  | O-C-N      | -5.32 | 115.99      | 122.22   |
| 18  | B     | 1147 | ASP  | CA-C-N     | 5.32  | 128.03      | 120.53   |
| 18  | B     | 1147 | ASP  | C-N-CA     | 5.32  | 128.03      | 120.53   |
| 19  | 48    | 282  | GLU  | O-C-N      | -5.32 | 117.15      | 123.22   |
| 4   | T8    | 58   | ASP  | CA-C-N     | 5.32  | 127.67      | 120.38   |
| 4   | T8    | 58   | ASP  | C-N-CA     | 5.32  | 127.67      | 120.38   |
| 6   | O8    | 181  | GLU  | CA-C-N     | -5.32 | 113.06      | 122.26   |
| 6   | O8    | 181  | GLU  | C-N-CA     | -5.32 | 113.06      | 122.26   |
| 9   | K8    | 1155 | THR  | O-C-N      | -5.32 | 116.45      | 122.68   |
| 5   | P8    | 207  | HIS  | CA-C-N     | -5.32 | 114.28      | 119.76   |
| 5   | P8    | 207  | HIS  | C-N-CA     | -5.32 | 114.28      | 119.76   |
| 10  | C     | 1269 | PHE  | CA-C-N     | -5.32 | 114.90      | 122.77   |
| 10  | C     | 1269 | PHE  | C-N-CA     | -5.32 | 114.90      | 122.77   |
| 10  | C8    | 847  | ARG  | O-C-N      | -5.32 | 115.74      | 122.17   |
| 7   | Q16   | 65   | ASN  | O-C-N      | 5.32  | 126.03      | 121.30   |
| 7   | Q16   | 224  | GLY  | O-C-N      | -5.32 | 115.77      | 122.41   |
| 9   | K     | 1184 | HIS  | O-C-N      | -5.32 | 116.09      | 122.15   |
| 10  | C24   | 682  | SER  | CA-C-N     | 5.32  | 130.50      | 122.42   |
| 10  | C24   | 682  | SER  | C-N-CA     | 5.32  | 130.50      | 122.42   |
| 10  | C     | 847  | ARG  | O-C-N      | -5.32 | 115.74      | 122.17   |
| 10  | C8    | 653  | TYR  | O-C-N      | -5.32 | 115.21      | 121.32   |
| 10  | C32   | 1386 | ASP  | O-C-N      | 5.32  | 127.75      | 122.12   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12  | A48   | 449  | ASP  | O-C-N      | 5.32  | 127.75      | 122.12   |
| 5   | P16   | 1    | MET  | O-C-N      | -5.31 | 114.50      | 123.00   |
| 2   | M16   | 244  | PHE  | O-C-N      | -5.31 | 115.73      | 121.95   |
| 5   | P     | 146  | SER  | O-C-N      | -5.31 | 115.53      | 122.59   |
| 6   | O16   | 181  | GLU  | CA-C-N     | -5.31 | 113.07      | 122.26   |
| 6   | O16   | 181  | GLU  | C-N-CA     | -5.31 | 113.07      | 122.26   |
| 10  | C24   | 1269 | PHE  | CA-C-N     | -5.31 | 114.91      | 122.77   |
| 10  | C24   | 1269 | PHE  | C-N-CA     | -5.31 | 114.91      | 122.77   |
| 11  | A16   | 834  | ARG  | O-C-N      | 5.31  | 127.75      | 122.12   |
| 18  | B8    | 465  | GLU  | O-C-N      | 5.31  | 128.21      | 122.15   |
| 18  | B8    | 1147 | ASP  | CA-C-N     | 5.31  | 128.02      | 120.53   |
| 18  | B8    | 1147 | ASP  | C-N-CA     | 5.31  | 128.02      | 120.53   |
| 10  | C32   | 1806 | ARG  | CA-C-N     | 5.31  | 127.93      | 120.28   |
| 10  | C32   | 1806 | ARG  | C-N-CA     | 5.31  | 127.93      | 120.28   |
| 12  | A     | 462  | THR  | CA-C-N     | 5.31  | 131.82      | 121.41   |
| 12  | A     | 462  | THR  | C-N-CA     | 5.31  | 131.82      | 121.41   |
| 10  | C     | 1771 | GLN  | CA-C-N     | 5.31  | 130.77      | 122.17   |
| 10  | C     | 1771 | GLN  | C-N-CA     | 5.31  | 130.77      | 122.17   |
| 10  | C32   | 152  | ILE  | O-C-N      | 5.31  | 127.02      | 121.87   |
| 1   | R     | 1440 | PRO  | CA-C-N     | 5.31  | 128.38      | 120.31   |
| 1   | R     | 1440 | PRO  | C-N-CA     | 5.31  | 128.38      | 120.31   |
| 2   | M16   | 203  | PRO  | O-C-N      | -5.31 | 116.15      | 122.89   |
| 10  | C16   | 1177 | ARG  | O-C-N      | 5.31  | 127.75      | 122.12   |
| 10  | C16   | 1771 | GLN  | CA-C-N     | 5.31  | 130.77      | 122.17   |
| 10  | C16   | 1771 | GLN  | C-N-CA     | 5.31  | 130.77      | 122.17   |
| 18  | B8    | 115  | THR  | CA-C-N     | -5.31 | 114.61      | 122.41   |
| 18  | B8    | 115  | THR  | C-N-CA     | -5.31 | 114.61      | 122.41   |
| 18  | B8    | 1264 | GLN  | O-C-N      | 5.31  | 127.75      | 122.12   |
| 19  | 4     | 372  | LYS  | CA-C-N     | -5.31 | 113.27      | 121.45   |
| 19  | 4     | 372  | LYS  | C-N-CA     | -5.31 | 113.27      | 121.45   |
| 23  | J32   | 723  | GLN  | O-C-N      | -5.31 | 115.31      | 122.43   |
| 24  | D8    | 681  | ASP  | CA-C-N     | 5.31  | 131.68      | 121.54   |
| 24  | D8    | 681  | ASP  | C-N-CA     | 5.31  | 131.68      | 121.54   |
| 24  | D32   | 745  | GLY  | CA-C-N     | 5.31  | 131.68      | 121.54   |
| 24  | D32   | 745  | GLY  | C-N-CA     | 5.31  | 131.68      | 121.54   |
| 5   | P     | 1    | MET  | O-C-N      | -5.31 | 114.51      | 123.00   |
| 8   | L16   | 315  | GLN  | OE1-CD-NE2 | -5.31 | 117.29      | 122.60   |
| 10  | C16   | 682  | SER  | CA-C-N     | 5.31  | 130.49      | 122.42   |
| 10  | C16   | 682  | SER  | C-N-CA     | 5.31  | 130.49      | 122.42   |
| 18  | B     | 465  | GLU  | O-C-N      | 5.31  | 128.20      | 122.15   |
| 10  | C32   | 667  | ILE  | O-C-N      | 5.31  | 127.80      | 121.80   |
| 10  | C16   | 43   | LEU  | CA-C-N     | 5.31  | 131.38      | 123.05   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C16   | 43   | LEU  | C-N-CA | 5.31  | 131.38      | 123.05   |
| 10  | C16   | 1078 | GLY  | O-C-N  | -5.31 | 115.80      | 122.70   |
| 11  | A24   | 449  | ASP  | O-C-N  | 5.31  | 127.74      | 122.12   |
| 10  | C24   | 1386 | ASP  | O-C-N  | 5.31  | 127.74      | 122.12   |
| 12  | A     | 834  | ARG  | O-C-N  | 5.31  | 127.74      | 122.12   |
| 22  | I     | 356  | ARG  | O-C-N  | 5.31  | 127.74      | 122.12   |
| 10  | C24   | 1729 | ASN  | CA-C-N | 5.30  | 128.85      | 120.47   |
| 10  | C24   | 1729 | ASN  | C-N-CA | 5.30  | 128.85      | 120.47   |
| 10  | C     | 1806 | ARG  | CA-C-N | 5.30  | 127.92      | 120.28   |
| 10  | C     | 1806 | ARG  | C-N-CA | 5.30  | 127.92      | 120.28   |
| 10  | C32   | 1076 | TYR  | CA-C-N | -5.30 | 113.47      | 121.05   |
| 10  | C32   | 1076 | TYR  | C-N-CA | -5.30 | 113.47      | 121.05   |
| 10  | C24   | 1771 | GLN  | CA-C-N | 5.30  | 130.76      | 122.17   |
| 10  | C24   | 1771 | GLN  | C-N-CA | 5.30  | 130.76      | 122.17   |
| 20  | E8    | 347  | PRO  | C-N-CD | -5.30 | 103.26      | 125.00   |
| 10  | C32   | 1078 | GLY  | O-C-N  | -5.30 | 115.81      | 122.70   |
| 6   | O     | 181  | GLU  | CA-C-N | -5.30 | 113.09      | 122.26   |
| 6   | O     | 181  | GLU  | C-N-CA | -5.30 | 113.09      | 122.26   |
| 10  | C16   | 653  | TYR  | O-C-N  | -5.30 | 115.23      | 121.32   |
| 10  | C24   | 1795 | ASP  | O-C-N  | -5.30 | 116.11      | 122.15   |
| 11  | A16   | 38   | ASP  | O-C-N  | 5.30  | 127.74      | 122.12   |
| 11  | A32   | 449  | ASP  | O-C-N  | 5.30  | 127.74      | 122.12   |
| 24  | D     | 681  | ASP  | CA-C-N | 5.30  | 131.66      | 121.54   |
| 24  | D     | 681  | ASP  | C-N-CA | 5.30  | 131.66      | 121.54   |
| 18  | B     | 485  | ASN  | O-C-N  | 5.30  | 127.73      | 122.12   |
| 4   | T16   | 58   | ASP  | CA-C-N | 5.30  | 127.64      | 120.38   |
| 4   | T16   | 58   | ASP  | C-N-CA | 5.30  | 127.64      | 120.38   |
| 10  | C8    | 115  | ILE  | O-C-N  | 5.30  | 127.01      | 121.87   |
| 10  | C8    | 682  | SER  | CA-C-N | 5.30  | 130.47      | 122.42   |
| 10  | C8    | 682  | SER  | C-N-CA | 5.30  | 130.47      | 122.42   |
| 18  | B     | 202  | LEU  | O-C-N  | 5.30  | 127.73      | 122.12   |
| 19  | 4     | 34   | TYR  | CA-C-N | 5.30  | 125.86      | 119.98   |
| 19  | 4     | 34   | TYR  | C-N-CA | 5.30  | 125.86      | 119.98   |
| 19  | 4     | 417  | ASP  | O-C-N  | -5.29 | 116.08      | 122.65   |
| 5   | P16   | 582  | GLU  | O-C-N  | 5.29  | 127.73      | 122.12   |
| 10  | C16   | 861  | ILE  | O-C-N  | -5.29 | 115.95      | 122.57   |
| 10  | C8    | 1538 | THR  | O-C-N  | -5.29 | 116.03      | 122.22   |
| 20  | E     | 347  | PRO  | C-N-CD | -5.29 | 103.29      | 125.00   |
| 23  | J32   | 684  | ASP  | O-C-N  | -5.29 | 115.47      | 122.57   |
| 10  | C32   | 847  | ARG  | O-C-N  | -5.29 | 115.76      | 122.17   |
| 10  | C32   | 1771 | GLN  | CA-C-N | 5.29  | 130.75      | 122.17   |
| 10  | C32   | 1771 | GLN  | C-N-CA | 5.29  | 130.75      | 122.17   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | C8    | 1340 | PRO  | CA-C-N | 5.29  | 128.11      | 120.38   |
| 10  | C8    | 1340 | PRO  | C-N-CA | 5.29  | 128.11      | 120.38   |
| 24  | D16   | 681  | ASP  | CA-C-N | 5.29  | 131.65      | 121.54   |
| 24  | D16   | 681  | ASP  | C-N-CA | 5.29  | 131.65      | 121.54   |
| 5   | P8    | 582  | GLU  | O-C-N  | 5.29  | 127.73      | 122.12   |
| 10  | C16   | 667  | ILE  | O-C-N  | 5.29  | 127.78      | 121.80   |
| 10  | C24   | 991  | LEU  | O-C-N  | 5.29  | 128.18      | 122.15   |
| 18  | B     | 1190 | GLY  | O-C-N  | -5.29 | 117.57      | 122.86   |
| 24  | D40   | 681  | ASP  | CA-C-N | 5.29  | 131.64      | 121.54   |
| 24  | D40   | 681  | ASP  | C-N-CA | 5.29  | 131.64      | 121.54   |
| 1   | R16   | 1440 | PRO  | CA-C-N | 5.29  | 128.35      | 120.31   |
| 1   | R16   | 1440 | PRO  | C-N-CA | 5.29  | 128.35      | 120.31   |
| 7   | Q     | 224  | GLY  | O-C-N  | -5.29 | 115.80      | 122.41   |
| 10  | C24   | 667  | ILE  | O-C-N  | 5.29  | 127.78      | 121.80   |
| 10  | C24   | 847  | ARG  | O-C-N  | -5.29 | 115.77      | 122.17   |
| 10  | C8    | 1269 | PHE  | CA-C-N | -5.29 | 114.94      | 122.77   |
| 10  | C8    | 1269 | PHE  | C-N-CA | -5.29 | 114.94      | 122.77   |
| 10  | C16   | 152  | ILE  | O-C-N  | 5.29  | 127.00      | 121.87   |
| 10  | C16   | 847  | ARG  | O-C-N  | -5.29 | 115.77      | 122.17   |
| 5   | P8    | 1    | MET  | O-C-N  | -5.29 | 114.54      | 123.00   |
| 10  | C24   | 72   | LEU  | O-C-N  | -5.29 | 117.30      | 123.27   |
| 14  | W     | 641  | GLU  | CA-C-N | 5.29  | 127.80      | 120.29   |
| 14  | W     | 641  | GLU  | C-N-CA | 5.29  | 127.80      | 120.29   |
| 10  | C8    | 533  | ALA  | O-C-N  | -5.29 | 117.05      | 123.13   |
| 2   | M16   | 531  | ASP  | O-C-N  | -5.28 | 115.61      | 122.37   |
| 10  | C16   | 1257 | ALA  | O-C-N  | 5.28  | 127.72      | 122.12   |
| 19  | 48    | 34   | TYR  | CA-C-N | 5.28  | 125.84      | 119.98   |
| 19  | 48    | 34   | TYR  | C-N-CA | 5.28  | 125.84      | 119.98   |
| 10  | C32   | 847  | ARG  | CA-C-N | 5.28  | 129.05      | 120.60   |
| 10  | C32   | 847  | ARG  | C-N-CA | 5.28  | 129.05      | 120.60   |
| 12  | A48   | 782  | PRO  | CA-C-N | 5.28  | 131.63      | 121.54   |
| 12  | A48   | 782  | PRO  | C-N-CA | 5.28  | 131.63      | 121.54   |
| 2   | M8    | 203  | PRO  | O-C-N  | -5.28 | 116.18      | 122.89   |
| 7   | Q     | 161  | LYS  | CA-C-N | -5.28 | 115.77      | 122.37   |
| 7   | Q     | 161  | LYS  | C-N-CA | -5.28 | 115.77      | 122.37   |
| 10  | C24   | 1491 | CYS  | O-C-N  | -5.28 | 115.64      | 122.77   |
| 11  | A40   | 157  | LEU  | O-C-N  | 5.28  | 125.95      | 121.20   |
| 10  | C16   | 1076 | TYR  | CA-C-N | -5.28 | 113.50      | 121.05   |
| 10  | C16   | 1076 | TYR  | C-N-CA | -5.28 | 113.50      | 121.05   |
| 10  | C24   | 1078 | GLY  | O-C-N  | -5.28 | 115.84      | 122.70   |
| 24  | D16   | 760  | SER  | CA-C-N | 5.28  | 131.62      | 121.54   |
| 24  | D16   | 760  | SER  | C-N-CA | 5.28  | 131.62      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12  | A48   | 639  | GLY  | O-C-N      | 5.28  | 127.26      | 122.88   |
| 1   | R     | 1203 | SER  | CA-C-N     | -5.28 | 111.46      | 121.54   |
| 1   | R     | 1203 | SER  | C-N-CA     | -5.28 | 111.46      | 121.54   |
| 14  | W     | 444  | ARG  | CD-NE-CZ   | 5.28  | 131.79      | 124.40   |
| 2   | M     | 203  | PRO  | O-C-N      | -5.28 | 116.19      | 122.89   |
| 10  | C8    | 847  | ARG  | CA-C-N     | 5.28  | 129.04      | 120.60   |
| 10  | C8    | 847  | ARG  | C-N-CA     | 5.28  | 129.04      | 120.60   |
| 19  | 48    | 28   | GLU  | O-C-N      | 5.28  | 127.51      | 122.07   |
| 24  | D8    | 760  | SER  | CA-C-N     | 5.28  | 131.62      | 121.54   |
| 24  | D8    | 760  | SER  | C-N-CA     | 5.28  | 131.62      | 121.54   |
| 10  | C16   | 1340 | PRO  | CA-C-N     | 5.28  | 128.08      | 120.38   |
| 10  | C16   | 1340 | PRO  | C-N-CA     | 5.28  | 128.08      | 120.38   |
| 10  | C24   | 1538 | THR  | O-C-N      | -5.28 | 116.05      | 122.22   |
| 12  | A     | 782  | PRO  | CA-C-N     | 5.28  | 131.62      | 121.54   |
| 12  | A     | 782  | PRO  | C-N-CA     | 5.28  | 131.62      | 121.54   |
| 24  | D32   | 760  | SER  | CA-C-N     | 5.28  | 131.62      | 121.54   |
| 24  | D32   | 760  | SER  | C-N-CA     | 5.28  | 131.62      | 121.54   |
| 10  | C32   | 1269 | PHE  | CA-C-N     | -5.28 | 114.96      | 122.77   |
| 10  | C32   | 1269 | PHE  | C-N-CA     | -5.28 | 114.96      | 122.77   |
| 10  | C24   | 1076 | TYR  | CA-C-N     | -5.27 | 113.51      | 121.05   |
| 10  | C24   | 1076 | TYR  | C-N-CA     | -5.27 | 113.51      | 121.05   |
| 19  | 4     | 24   | ASN  | CA-C-N     | -5.27 | 114.07      | 121.72   |
| 19  | 4     | 24   | ASN  | C-N-CA     | -5.27 | 114.07      | 121.72   |
| 8   | L     | 315  | GLN  | OE1-CD-NE2 | -5.27 | 117.33      | 122.60   |
| 10  | C     | 861  | ILE  | O-C-N      | -5.27 | 115.98      | 122.57   |
| 18  | B     | 115  | THR  | CA-C-N     | -5.27 | 114.66      | 122.41   |
| 18  | B     | 115  | THR  | C-N-CA     | -5.27 | 114.66      | 122.41   |
| 10  | C16   | 72   | LEU  | O-C-N      | -5.27 | 117.31      | 123.27   |
| 18  | B8    | 5    | ASN  | O-C-N      | -5.27 | 115.65      | 122.77   |
| 24  | D40   | 760  | SER  | CA-C-N     | 5.27  | 131.61      | 121.54   |
| 24  | D40   | 760  | SER  | C-N-CA     | 5.27  | 131.61      | 121.54   |
| 10  | C24   | 1257 | ALA  | O-C-N      | 5.27  | 127.71      | 122.12   |
| 11  | A40   | 449  | ASP  | O-C-N      | 5.27  | 127.71      | 122.12   |
| 10  | C8    | 1729 | ASN  | CA-C-N     | 5.27  | 128.80      | 120.47   |
| 10  | C8    | 1729 | ASN  | C-N-CA     | 5.27  | 128.80      | 120.47   |
| 18  | B8    | 1685 | THR  | O-C-N      | -5.27 | 116.34      | 123.19   |
| 10  | C32   | 1177 | ARG  | O-C-N      | 5.27  | 127.70      | 122.12   |
| 10  | C32   | 1795 | ASP  | O-C-N      | -5.27 | 116.14      | 122.15   |
| 1   | R8    | 1203 | SER  | CA-C-N     | -5.27 | 111.48      | 121.54   |
| 1   | R8    | 1203 | SER  | C-N-CA     | -5.27 | 111.48      | 121.54   |
| 5   | P8    | 146  | SER  | O-C-N      | -5.27 | 115.58      | 122.59   |
| 5   | P16   | 207  | HIS  | CA-C-N     | -5.27 | 114.33      | 119.76   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | P16   | 207  | HIS  | C-N-CA | -5.27 | 114.33      | 119.76   |
| 9   | K     | 1160 | ARG  | O-C-N  | 5.27  | 128.75      | 122.27   |
| 11  | A16   | 525  | ALA  | O-C-N  | -5.27 | 115.58      | 122.59   |
| 18  | B8    | 1190 | GLY  | O-C-N  | -5.27 | 117.59      | 122.86   |
| 19  | 4     | 28   | GLU  | O-C-N  | 5.27  | 127.50      | 122.07   |
| 24  | D     | 760  | SER  | CA-C-N | 5.27  | 131.60      | 121.54   |
| 24  | D     | 760  | SER  | C-N-CA | 5.27  | 131.60      | 121.54   |
| 12  | A     | 157  | LEU  | O-C-N  | 5.27  | 125.94      | 121.20   |
| 18  | B     | 693  | SER  | CA-C-N | 5.27  | 131.73      | 121.41   |
| 18  | B     | 693  | SER  | C-N-CA | 5.27  | 131.73      | 121.41   |
| 4   | T     | 58   | ASP  | CA-C-N | 5.26  | 127.59      | 120.38   |
| 4   | T     | 58   | ASP  | C-N-CA | 5.26  | 127.59      | 120.38   |
| 5   | P16   | 146  | SER  | O-C-N  | -5.26 | 115.59      | 122.59   |
| 5   | P16   | 446  | HIS  | CA-C-N | -5.26 | 113.58      | 120.95   |
| 5   | P16   | 446  | HIS  | C-N-CA | -5.26 | 113.58      | 120.95   |
| 10  | C     | 682  | SER  | CA-C-N | 5.26  | 130.42      | 122.42   |
| 10  | C     | 682  | SER  | C-N-CA | 5.26  | 130.42      | 122.42   |
| 10  | C16   | 1538 | THR  | O-C-N  | -5.26 | 116.06      | 122.22   |
| 12  | A48   | 140  | TRP  | O-C-N  | -5.26 | 116.15      | 122.15   |
| 6   | O     | 37   | GLU  | O-C-N  | 5.26  | 129.54      | 123.17   |
| 10  | C16   | 1780 | ARG  | O-C-N  | -5.26 | 115.59      | 122.59   |
| 11  | A40   | 140  | TRP  | O-C-N  | -5.26 | 116.15      | 122.15   |
| 1   | R8    | 1440 | PRO  | CA-C-N | 5.26  | 128.30      | 120.31   |
| 1   | R8    | 1440 | PRO  | C-N-CA | 5.26  | 128.30      | 120.31   |
| 2   | M16   | 326  | GLN  | O-C-N  | -5.26 | 115.59      | 122.59   |
| 3   | N16   | 66   | HIS  | CA-C-N | 5.26  | 124.92      | 119.56   |
| 3   | N16   | 66   | HIS  | C-N-CA | 5.26  | 124.92      | 119.56   |
| 7   | Q8    | 224  | GLY  | O-C-N  | -5.26 | 115.84      | 122.41   |
| 19  | 48    | 24   | ASN  | CA-C-N | -5.26 | 114.09      | 121.72   |
| 19  | 48    | 24   | ASN  | C-N-CA | -5.26 | 114.09      | 121.72   |
| 10  | C32   | 931  | PRO  | O-C-N  | -5.26 | 115.19      | 122.24   |
| 2   | M8    | 326  | GLN  | O-C-N  | -5.26 | 115.60      | 122.59   |
| 11  | A40   | 525  | ALA  | O-C-N  | -5.26 | 115.60      | 122.59   |
| 10  | C8    | 1076 | TYR  | CA-C-N | -5.26 | 113.53      | 121.05   |
| 10  | C8    | 1076 | TYR  | C-N-CA | -5.26 | 113.53      | 121.05   |
| 16  | A8    | 157  | LEU  | O-C-N  | 5.26  | 125.93      | 121.20   |
| 22  | I24   | 348  | ASP  | CA-C-N | 5.26  | 125.06      | 119.28   |
| 22  | I24   | 348  | ASP  | C-N-CA | 5.26  | 125.06      | 119.28   |
| 10  | C32   | 1780 | ARG  | O-C-N  | -5.26 | 115.60      | 122.59   |
| 11  | A24   | 525  | ALA  | O-C-N  | -5.25 | 115.60      | 122.59   |
| 10  | C8    | 667  | ILE  | O-C-N  | 5.25  | 127.73      | 121.80   |
| 18  | B     | 5    | ASN  | O-C-N  | -5.25 | 115.68      | 122.77   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B     | 1247 | GLY  | O-C-N      | 5.25  | 127.23      | 122.19   |
| 14  | W     | 49   | GLN  | OE1-CD-NE2 | -5.25 | 117.35      | 122.60   |
| 18  | B8    | 693  | SER  | CA-C-N     | 5.25  | 131.70      | 121.41   |
| 18  | B8    | 693  | SER  | C-N-CA     | 5.25  | 131.70      | 121.41   |
| 1   | R16   | 1203 | SER  | CA-C-N     | -5.25 | 111.52      | 121.54   |
| 1   | R16   | 1203 | SER  | C-N-CA     | -5.25 | 111.52      | 121.54   |
| 10  | C     | 1076 | TYR  | CA-C-N     | -5.25 | 113.55      | 121.05   |
| 10  | C     | 1076 | TYR  | C-N-CA     | -5.25 | 113.55      | 121.05   |
| 10  | C8    | 1716 | LYS  | O-C-N      | 5.25  | 128.13      | 122.15   |
| 18  | B     | 1013 | VAL  | O-C-N      | -5.25 | 116.57      | 121.87   |
| 18  | B8    | 675  | SER  | CA-C-N     | -5.25 | 112.72      | 120.28   |
| 18  | B8    | 675  | SER  | C-N-CA     | -5.25 | 112.72      | 120.28   |
| 10  | C16   | 1269 | PHE  | CA-C-N     | -5.25 | 115.00      | 122.77   |
| 10  | C16   | 1269 | PHE  | C-N-CA     | -5.25 | 115.00      | 122.77   |
| 11  | A40   | 834  | ARG  | O-C-N      | 5.25  | 127.68      | 122.12   |
| 13  | V     | 888  | PRO  | O-C-N      | -5.25 | 116.45      | 122.85   |
| 10  | C     | 1078 | GLY  | O-C-N      | -5.25 | 115.88      | 122.70   |
| 19  | 48    | 417  | ASP  | O-C-N      | -5.25 | 116.14      | 122.65   |
| 2   | M8    | 531  | ASP  | O-C-N      | -5.24 | 115.66      | 122.37   |
| 6   | O16   | 37   | GLU  | O-C-N      | 5.24  | 129.51      | 123.17   |
| 10  | C     | 1780 | ARG  | O-C-N      | -5.24 | 115.62      | 122.59   |
| 10  | C32   | 861  | ILE  | O-C-N      | -5.24 | 116.02      | 122.57   |
| 7   | Q8    | 161  | LYS  | CA-C-N     | -5.24 | 115.82      | 122.37   |
| 7   | Q8    | 161  | LYS  | C-N-CA     | -5.24 | 115.82      | 122.37   |
| 8   | L8    | 315  | GLN  | OE1-CD-NE2 | -5.24 | 117.36      | 122.60   |
| 10  | C24   | 378  | GLU  | O-C-N      | -5.24 | 116.42      | 122.87   |
| 12  | A     | 639  | GLY  | O-C-N      | 5.24  | 127.23      | 122.88   |
| 10  | C     | 72   | LEU  | O-C-N      | -5.24 | 117.35      | 123.27   |
| 10  | C8    | 1078 | GLY  | O-C-N      | -5.24 | 115.89      | 122.70   |
| 10  | C32   | 378  | GLU  | O-C-N      | -5.24 | 116.42      | 122.87   |
| 12  | A48   | 525  | ALA  | O-C-N      | -5.24 | 115.62      | 122.59   |
| 12  | A48   | 558  | SER  | O-C-N      | -5.24 | 116.58      | 122.97   |
| 9   | K8    | 828  | PRO  | O-C-N      | -5.24 | 116.57      | 122.91   |
| 11  | A24   | 834  | ARG  | O-C-N      | 5.24  | 127.67      | 122.12   |
| 12  | A     | 525  | ALA  | O-C-N      | -5.24 | 115.62      | 122.59   |
| 10  | C     | 1332 | GLN  | O-C-N      | -5.24 | 116.09      | 122.22   |
| 11  | A24   | 639  | GLY  | O-C-N      | 5.24  | 127.23      | 122.88   |
| 10  | C24   | 1363 | ASP  | O-C-N      | 5.24  | 127.67      | 122.12   |
| 10  | C24   | 1780 | ARG  | O-C-N      | -5.24 | 115.62      | 122.59   |
| 10  | C32   | 1257 | ALA  | O-C-N      | 5.24  | 127.67      | 122.12   |
| 13  | V     | 859  | ARG  | O-C-N      | 5.24  | 127.67      | 122.12   |
| 11  | A24   | 782  | PRO  | CA-C-N     | 5.23  | 131.54      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | A24   | 782  | PRO  | C-N-CA   | 5.23  | 131.54      | 121.54   |
| 10  | C24   | 931  | PRO  | O-C-N    | -5.23 | 115.23      | 122.24   |
| 18  | B     | 675  | SER  | CA-C-N   | -5.23 | 112.74      | 120.28   |
| 18  | B     | 675  | SER  | C-N-CA   | -5.23 | 112.74      | 120.28   |
| 18  | B8    | 1247 | GLY  | O-C-N    | 5.23  | 127.21      | 122.19   |
| 10  | C8    | 72   | LEU  | O-C-N    | -5.23 | 117.36      | 123.27   |
| 11  | A32   | 525  | ALA  | O-C-N    | -5.23 | 115.63      | 122.59   |
| 8   | L     | 297  | ASP  | CA-CB-CG | 5.23  | 117.83      | 112.60   |
| 8   | L16   | 297  | ASP  | CA-CB-CG | 5.23  | 117.83      | 112.60   |
| 9   | K8    | 1160 | ARG  | O-C-N    | 5.23  | 128.70      | 122.27   |
| 10  | C16   | 759  | VAL  | O-C-N    | -5.23 | 116.59      | 121.87   |
| 10  | C16   | 1729 | ASN  | CA-C-N   | 5.23  | 128.73      | 120.47   |
| 10  | C16   | 1729 | ASN  | C-N-CA   | 5.23  | 128.73      | 120.47   |
| 12  | A     | 558  | SER  | O-C-N    | -5.23 | 116.59      | 122.97   |
| 11  | A40   | 782  | PRO  | CA-C-N   | 5.23  | 131.53      | 121.54   |
| 11  | A40   | 782  | PRO  | C-N-CA   | 5.23  | 131.53      | 121.54   |
| 10  | C     | 378  | GLU  | O-C-N    | -5.23 | 116.44      | 122.87   |
| 22  | I24   | 356  | ARG  | O-C-N    | 5.23  | 127.66      | 122.12   |
| 24  | D24   | 760  | SER  | CA-C-N   | 5.23  | 131.53      | 121.54   |
| 24  | D24   | 760  | SER  | C-N-CA   | 5.23  | 131.53      | 121.54   |
| 6   | O8    | 37   | GLU  | O-C-N    | 5.23  | 129.50      | 123.17   |
| 10  | C24   | 1383 | GLY  | O-C-N    | -5.23 | 117.17      | 122.19   |
| 22  | I8    | 97   | THR  | CA-C-N   | 5.23  | 128.96      | 120.60   |
| 22  | I8    | 97   | THR  | C-N-CA   | 5.23  | 128.96      | 120.60   |
| 5   | P     | 446  | HIS  | CA-C-N   | -5.23 | 113.63      | 120.95   |
| 5   | P     | 446  | HIS  | C-N-CA   | -5.23 | 113.63      | 120.95   |
| 16  | A8    | 140  | TRP  | O-C-N    | -5.23 | 116.19      | 122.15   |
| 18  | B     | 1443 | SER  | CA-C-N   | -5.23 | 113.51      | 121.66   |
| 18  | B     | 1443 | SER  | C-N-CA   | -5.23 | 113.51      | 121.66   |
| 3   | N16   | 160  | PRO  | O-C-N    | -5.22 | 116.53      | 123.01   |
| 10  | C16   | 1059 | ALA  | CA-C-N   | -5.22 | 113.81      | 122.32   |
| 10  | C16   | 1059 | ALA  | C-N-CA   | -5.22 | 113.81      | 122.32   |
| 10  | C16   | 1716 | LYS  | O-C-N    | 5.22  | 128.11      | 122.15   |
| 22  | I     | 97   | THR  | CA-C-N   | 5.22  | 128.96      | 120.60   |
| 22  | I     | 97   | THR  | C-N-CA   | 5.22  | 128.96      | 120.60   |
| 22  | I16   | 97   | THR  | CA-C-N   | 5.22  | 128.96      | 120.60   |
| 22  | I16   | 97   | THR  | C-N-CA   | 5.22  | 128.96      | 120.60   |
| 3   | N     | 160  | PRO  | O-C-N    | -5.22 | 116.53      | 123.01   |
| 10  | C16   | 578  | LEU  | CA-C-N   | 5.22  | 128.25      | 120.31   |
| 10  | C16   | 578  | LEU  | C-N-CA   | 5.22  | 128.25      | 120.31   |
| 10  | C16   | 931  | PRO  | O-C-N    | -5.22 | 115.24      | 122.24   |
| 11  | A24   | 140  | TRP  | O-C-N    | -5.22 | 116.20      | 122.15   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 6   | O16   | 93   | HIS  | CA-C-N    | 5.22  | 131.64      | 121.41   |
| 6   | O16   | 93   | HIS  | C-N-CA    | 5.22  | 131.64      | 121.41   |
| 5   | P     | 582  | GLU  | O-C-N     | 5.22  | 127.65      | 122.12   |
| 5   | P16   | 391  | LYS  | CA-C-N    | -5.22 | 113.31      | 119.84   |
| 5   | P16   | 391  | LYS  | C-N-CA    | -5.22 | 113.31      | 119.84   |
| 9   | K     | 828  | PRO  | O-C-N     | -5.22 | 116.59      | 122.91   |
| 10  | C32   | 1729 | ASN  | CA-C-N    | 5.22  | 128.72      | 120.47   |
| 10  | C32   | 1729 | ASN  | C-N-CA    | 5.22  | 128.72      | 120.47   |
| 10  | C     | 1729 | ASN  | CA-C-N    | 5.22  | 128.71      | 120.47   |
| 10  | C     | 1729 | ASN  | C-N-CA    | 5.22  | 128.71      | 120.47   |
| 5   | P8    | 446  | HIS  | CA-C-N    | -5.22 | 113.65      | 120.95   |
| 5   | P8    | 446  | HIS  | C-N-CA    | -5.22 | 113.65      | 120.95   |
| 10  | C     | 759  | VAL  | O-C-N     | -5.22 | 116.60      | 121.87   |
| 18  | B8    | 1068 | THR  | CA-C-N    | 5.22  | 131.36      | 121.97   |
| 18  | B8    | 1068 | THR  | C-N-CA    | 5.22  | 131.36      | 121.97   |
| 10  | C16   | 729  | SER  | CA-C-N    | 5.21  | 131.50      | 121.54   |
| 10  | C16   | 729  | SER  | C-N-CA    | 5.21  | 131.50      | 121.54   |
| 10  | C24   | 1059 | ALA  | CA-C-N    | -5.21 | 113.82      | 122.32   |
| 10  | C24   | 1059 | ALA  | C-N-CA    | -5.21 | 113.82      | 122.32   |
| 10  | C32   | 72   | LEU  | O-C-N     | -5.21 | 117.38      | 123.27   |
| 3   | N8    | 160  | PRO  | O-C-N     | -5.21 | 116.55      | 123.01   |
| 10  | C     | 169  | GLN  | O-C-N     | 5.21  | 127.64      | 122.12   |
| 11  | A32   | 463  | GLY  | CA-C-N    | -5.21 | 114.27      | 120.00   |
| 11  | A32   | 463  | GLY  | C-N-CA    | -5.21 | 114.27      | 120.00   |
| 18  | B     | 1685 | THR  | O-C-N     | -5.21 | 116.41      | 123.19   |
| 18  | B8    | 1443 | SER  | CA-C-N    | -5.21 | 113.53      | 121.66   |
| 18  | B8    | 1443 | SER  | C-N-CA    | -5.21 | 113.53      | 121.66   |
| 10  | C8    | 1780 | ARG  | O-C-N     | -5.21 | 115.66      | 122.59   |
| 22  | I     | 133  | GLU  | CA-C-N    | 5.21  | 127.26      | 120.28   |
| 22  | I     | 133  | GLU  | C-N-CA    | 5.21  | 127.26      | 120.28   |
| 22  | I24   | 97   | THR  | CA-C-N    | 5.21  | 128.94      | 120.60   |
| 22  | I24   | 97   | THR  | C-N-CA    | 5.21  | 128.94      | 120.60   |
| 11  | A32   | 782  | PRO  | CA-C-N    | 5.21  | 131.49      | 121.54   |
| 11  | A32   | 782  | PRO  | C-N-CA    | 5.21  | 131.49      | 121.54   |
| 1   | R8    | 395  | HIS  | CB-CG-CD2 | -5.21 | 124.43      | 131.20   |
| 2   | M16   | 204  | ILE  | CA-C-N    | 5.21  | 131.11      | 122.73   |
| 2   | M16   | 204  | ILE  | C-N-CA    | 5.21  | 131.11      | 122.73   |
| 15  | J     | 704  | MET  | O-C-N     | 5.21  | 128.08      | 122.15   |
| 10  | C8    | 378  | GLU  | O-C-N     | -5.21 | 116.47      | 122.87   |
| 10  | C8    | 1059 | ALA  | CA-C-N    | -5.21 | 113.84      | 122.32   |
| 10  | C8    | 1059 | ALA  | C-N-CA    | -5.21 | 113.84      | 122.32   |
| 22  | I8    | 133  | GLU  | CA-C-N    | 5.21  | 127.25      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22  | I8    | 133  | GLU  | C-N-CA | 5.21  | 127.25      | 120.28   |
| 10  | C24   | 729  | SER  | CA-C-N | 5.20  | 131.48      | 121.54   |
| 10  | C24   | 729  | SER  | C-N-CA | 5.20  | 131.48      | 121.54   |
| 10  | C8    | 1257 | ALA  | O-C-N  | 5.20  | 127.64      | 122.12   |
| 7   | Q16   | 269  | VAL  | O-C-N  | -5.20 | 117.00      | 122.67   |
| 10  | C16   | 378  | GLU  | O-C-N  | -5.20 | 116.47      | 122.87   |
| 18  | B     | 913  | SER  | O-C-N  | -5.20 | 115.19      | 122.37   |
| 2   | M     | 531  | ASP  | O-C-N  | -5.20 | 115.71      | 122.37   |
| 18  | B     | 1790 | ALA  | CA-C-N | -5.20 | 112.61      | 121.97   |
| 18  | B     | 1790 | ALA  | C-N-CA | -5.20 | 112.61      | 121.97   |
| 23  | J32   | 614  | ASP  | O-C-N  | 5.20  | 127.63      | 122.12   |
| 11  | A24   | 463  | GLY  | CA-C-N | -5.20 | 114.28      | 120.00   |
| 11  | A24   | 463  | GLY  | C-N-CA | -5.20 | 114.28      | 120.00   |
| 10  | C32   | 1716 | LYS  | O-C-N  | 5.20  | 128.08      | 122.15   |
| 5   | P8    | 391  | LYS  | CA-C-N | -5.20 | 113.34      | 119.84   |
| 5   | P8    | 391  | LYS  | C-N-CA | -5.20 | 113.34      | 119.84   |
| 7   | Q16   | 161  | LYS  | CA-C-N | -5.20 | 115.87      | 122.37   |
| 7   | Q16   | 161  | LYS  | C-N-CA | -5.20 | 115.87      | 122.37   |
| 11  | A16   | 782  | PRO  | CA-C-N | 5.20  | 131.47      | 121.54   |
| 11  | A16   | 782  | PRO  | C-N-CA | 5.20  | 131.47      | 121.54   |
| 2   | M     | 354  | ASP  | O-C-N  | -5.20 | 115.68      | 122.59   |
| 23  | J24   | 681  | GLU  | O-C-N  | -5.20 | 114.10      | 122.41   |
| 6   | O8    | 93   | HIS  | CA-C-N | 5.19  | 131.59      | 121.41   |
| 6   | O8    | 93   | HIS  | C-N-CA | 5.19  | 131.59      | 121.41   |
| 10  | C     | 931  | PRO  | O-C-N  | -5.19 | 115.28      | 122.24   |
| 22  | I16   | 348  | ASP  | CA-C-N | 5.19  | 124.99      | 119.28   |
| 22  | I16   | 348  | ASP  | C-N-CA | 5.19  | 124.99      | 119.28   |
| 10  | C32   | 729  | SER  | CA-C-N | 5.19  | 131.46      | 121.54   |
| 10  | C32   | 729  | SER  | C-N-CA | 5.19  | 131.46      | 121.54   |
| 2   | M     | 204  | ILE  | CA-C-N | 5.19  | 131.09      | 122.73   |
| 2   | M     | 204  | ILE  | C-N-CA | 5.19  | 131.09      | 122.73   |
| 10  | C8    | 759  | VAL  | O-C-N  | -5.19 | 116.63      | 121.87   |
| 18  | B     | 1068 | THR  | CA-C-N | 5.19  | 131.31      | 121.97   |
| 18  | B     | 1068 | THR  | C-N-CA | 5.19  | 131.31      | 121.97   |
| 19  | 4     | 95   | THR  | CA-C-N | -5.19 | 110.90      | 121.18   |
| 19  | 4     | 95   | THR  | C-N-CA | -5.19 | 110.90      | 121.18   |
| 18  | B8    | 504  | PRO  | O-C-N  | -5.19 | 115.64      | 122.64   |
| 18  | B8    | 1161 | LEU  | CA-C-N | -5.19 | 114.26      | 121.99   |
| 18  | B8    | 1161 | LEU  | C-N-CA | -5.19 | 114.26      | 121.99   |
| 10  | C24   | 861  | ILE  | O-C-N  | -5.19 | 116.09      | 122.57   |
| 11  | A40   | 45   | LYS  | O-C-N  | 5.19  | 127.62      | 122.12   |
| 10  | C     | 729  | SER  | CA-C-N | 5.19  | 131.45      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 10  | C     | 729  | SER  | C-N-CA    | 5.19  | 131.45      | 121.54   |
| 10  | C     | 1257 | ALA  | O-C-N     | 5.19  | 127.62      | 122.12   |
| 11  | A16   | 45   | LYS  | O-C-N     | 5.19  | 127.62      | 122.12   |
| 10  | C8    | 1290 | HIS  | CA-C-N    | -5.19 | 113.58      | 121.31   |
| 10  | C8    | 1290 | HIS  | C-N-CA    | -5.19 | 113.58      | 121.31   |
| 19  | 48    | 70   | SER  | O-C-N     | -5.19 | 114.86      | 122.43   |
| 5   | P     | 391  | LYS  | CA-C-N    | -5.18 | 113.36      | 119.84   |
| 5   | P     | 391  | LYS  | C-N-CA    | -5.18 | 113.36      | 119.84   |
| 10  | C16   | 662  | LEU  | O-C-N     | 5.18  | 127.62      | 122.12   |
| 10  | C     | 1080 | SER  | CA-C-N    | 5.18  | 131.44      | 121.54   |
| 10  | C     | 1080 | SER  | C-N-CA    | 5.18  | 131.44      | 121.54   |
| 22  | I     | 348  | ASP  | CA-C-N    | 5.18  | 124.98      | 119.28   |
| 22  | I     | 348  | ASP  | C-N-CA    | 5.18  | 124.98      | 119.28   |
| 2   | M16   | 551  | GLU  | O-C-N     | -5.18 | 114.71      | 123.00   |
| 11  | A24   | 45   | LYS  | O-C-N     | 5.18  | 127.61      | 122.12   |
| 11  | A40   | 463  | GLY  | CA-C-N    | -5.18 | 114.30      | 120.00   |
| 11  | A40   | 463  | GLY  | C-N-CA    | -5.18 | 114.30      | 120.00   |
| 10  | C     | 898  | GLN  | O-C-N     | 5.18  | 127.61      | 122.12   |
| 10  | C32   | 759  | VAL  | O-C-N     | -5.18 | 116.64      | 121.87   |
| 10  | C32   | 1080 | SER  | CA-C-N    | 5.18  | 131.44      | 121.54   |
| 10  | C32   | 1080 | SER  | C-N-CA    | 5.18  | 131.44      | 121.54   |
| 2   | M8    | 204  | ILE  | CA-C-N    | 5.18  | 131.07      | 122.73   |
| 2   | M8    | 204  | ILE  | C-N-CA    | 5.18  | 131.07      | 122.73   |
| 2   | M8    | 354  | ASP  | O-C-N     | -5.18 | 115.70      | 122.59   |
| 6   | O     | 93   | HIS  | CA-C-N    | 5.18  | 131.56      | 121.41   |
| 6   | O     | 93   | HIS  | C-N-CA    | 5.18  | 131.56      | 121.41   |
| 10  | C     | 1059 | ALA  | CA-C-N    | -5.18 | 113.88      | 122.32   |
| 10  | C     | 1059 | ALA  | C-N-CA    | -5.18 | 113.88      | 122.32   |
| 10  | C8    | 1383 | GLY  | O-C-N     | -5.18 | 117.22      | 122.19   |
| 11  | A16   | 463  | GLY  | CA-C-N    | -5.18 | 114.30      | 120.00   |
| 11  | A16   | 463  | GLY  | C-N-CA    | -5.18 | 114.30      | 120.00   |
| 11  | A32   | 45   | LYS  | O-C-N     | 5.18  | 127.61      | 122.12   |
| 10  | C32   | 1059 | ALA  | CA-C-N    | -5.18 | 113.88      | 122.32   |
| 10  | C32   | 1059 | ALA  | C-N-CA    | -5.18 | 113.88      | 122.32   |
| 10  | C24   | 662  | LEU  | O-C-N     | 5.18  | 127.61      | 122.12   |
| 23  | J32   | 681  | GLU  | O-C-N     | -5.18 | 114.12      | 122.41   |
| 22  | I24   | 133  | GLU  | CA-C-N    | 5.18  | 127.22      | 120.28   |
| 22  | I24   | 133  | GLU  | C-N-CA    | 5.18  | 127.22      | 120.28   |
| 10  | C     | 1383 | GLY  | O-C-N     | -5.18 | 117.22      | 122.19   |
| 18  | B8    | 913  | SER  | O-C-N     | -5.18 | 115.23      | 122.37   |
| 23  | J16   | 681  | GLU  | O-C-N     | -5.18 | 114.13      | 122.41   |
| 1   | R16   | 395  | HIS  | CB-CG-CD2 | -5.17 | 124.47      | 131.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | M16   | 288  | ILE  | O-C-N     | 5.17  | 126.89      | 121.87   |
| 10  | C24   | 1080 | SER  | CA-C-N    | 5.17  | 131.42      | 121.54   |
| 10  | C24   | 1080 | SER  | C-N-CA    | 5.17  | 131.42      | 121.54   |
| 19  | 48    | 95   | THR  | CA-C-N    | -5.17 | 110.94      | 121.18   |
| 19  | 48    | 95   | THR  | C-N-CA    | -5.17 | 110.94      | 121.18   |
| 23  | J8    | 614  | ASP  | O-C-N     | 5.17  | 127.61      | 122.12   |
| 18  | B8    | 1790 | ALA  | CA-C-N    | -5.17 | 112.66      | 121.97   |
| 18  | B8    | 1790 | ALA  | C-N-CA    | -5.17 | 112.66      | 121.97   |
| 23  | J16   | 614  | ASP  | O-C-N     | 5.17  | 127.60      | 122.12   |
| 12  | A48   | 463  | GLY  | CA-C-N    | -5.17 | 114.31      | 120.00   |
| 12  | A48   | 463  | GLY  | C-N-CA    | -5.17 | 114.31      | 120.00   |
| 22  | I16   | 133  | GLU  | CA-C-N    | 5.17  | 127.21      | 120.28   |
| 22  | I16   | 133  | GLU  | C-N-CA    | 5.17  | 127.21      | 120.28   |
| 2   | M16   | 328  | THR  | CA-C-N    | -5.17 | 113.30      | 120.38   |
| 2   | M16   | 328  | THR  | C-N-CA    | -5.17 | 113.30      | 120.38   |
| 10  | C16   | 1119 | GLU  | O-C-N     | 5.17  | 127.60      | 122.12   |
| 10  | C16   | 1514 | ASN  | O-C-N     | 5.17  | 128.63      | 122.27   |
| 6   | O8    | 120  | LYS  | CA-C-N    | -5.17 | 112.97      | 121.80   |
| 6   | O8    | 120  | LYS  | C-N-CA    | -5.17 | 112.97      | 121.80   |
| 11  | A32   | 558  | SER  | O-C-N     | -5.17 | 116.67      | 122.97   |
| 2   | M     | 538  | LEU  | O-C-N     | 5.17  | 127.59      | 122.12   |
| 18  | B8    | 134  | GLN  | O-C-N     | 5.17  | 128.04      | 122.15   |
| 5   | P     | 63   | ASP  | O-C-N     | -5.16 | 115.56      | 122.43   |
| 6   | O     | 120  | LYS  | CA-C-N    | -5.16 | 112.97      | 121.80   |
| 6   | O     | 120  | LYS  | C-N-CA    | -5.16 | 112.97      | 121.80   |
| 10  | C24   | 1716 | LYS  | O-C-N     | 5.16  | 128.04      | 122.15   |
| 10  | C8    | 1119 | GLU  | O-C-N     | 5.16  | 127.59      | 122.12   |
| 21  | H     | 325  | PRO  | O-C-N     | 5.16  | 129.15      | 122.85   |
| 24  | D32   | 320  | PRO  | N-CA-CB   | 5.16  | 107.84      | 103.35   |
| 10  | C8    | 1063 | PRO  | CA-C-N    | -5.16 | 111.68      | 121.54   |
| 10  | C8    | 1063 | PRO  | C-N-CA    | -5.16 | 111.68      | 121.54   |
| 18  | B8    | 1098 | MET  | O-C-N     | 5.16  | 128.03      | 122.15   |
| 19  | 4     | 70   | SER  | O-C-N     | -5.16 | 114.89      | 122.43   |
| 2   | M     | 551  | GLU  | O-C-N     | -5.16 | 114.74      | 123.00   |
| 8   | L8    | 297  | ASP  | CA-CB-CG  | 5.16  | 117.76      | 112.60   |
| 10  | C24   | 759  | VAL  | O-C-N     | -5.16 | 116.66      | 121.87   |
| 10  | C     | 1657 | SER  | CA-C-N    | 5.16  | 131.40      | 121.54   |
| 10  | C     | 1657 | SER  | C-N-CA    | 5.16  | 131.40      | 121.54   |
| 10  | C32   | 304  | GLY  | CA-C-N    | 5.16  | 129.34      | 120.72   |
| 10  | C32   | 304  | GLY  | C-N-CA    | 5.16  | 129.34      | 120.72   |
| 1   | R     | 395  | HIS  | CB-CG-CD2 | -5.16 | 124.49      | 131.20   |
| 2   | M8    | 551  | GLU  | O-C-N     | -5.16 | 114.75      | 123.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | P16   | 24   | VAL  | O-C-N      | -5.16 | 117.08      | 122.81   |
| 10  | C16   | 169  | GLN  | O-C-N      | 5.16  | 127.59      | 122.12   |
| 12  | A     | 463  | GLY  | CA-C-N     | -5.16 | 114.33      | 120.00   |
| 12  | A     | 463  | GLY  | C-N-CA     | -5.16 | 114.33      | 120.00   |
| 13  | V     | 777  | ALA  | O-C-N      | 5.16  | 127.59      | 122.12   |
| 10  | C8    | 1080 | SER  | CA-C-N     | 5.16  | 131.39      | 121.54   |
| 10  | C8    | 1080 | SER  | C-N-CA     | 5.16  | 131.39      | 121.54   |
| 18  | B     | 1161 | LEU  | CA-C-N     | -5.16 | 114.30      | 121.99   |
| 18  | B     | 1161 | LEU  | C-N-CA     | -5.16 | 114.30      | 121.99   |
| 23  | J8    | 681  | GLU  | O-C-N      | -5.16 | 114.16      | 122.41   |
| 1   | R     | 801  | PHE  | CB-CA-C    | -5.16 | 101.92      | 110.68   |
| 12  | A     | 140  | TRP  | O-C-N      | -5.16 | 116.27      | 122.15   |
| 19  | 48    | 375  | ASP  | CA-C-N     | 5.16  | 127.70      | 120.28   |
| 19  | 48    | 375  | ASP  | C-N-CA     | 5.16  | 127.70      | 120.28   |
| 22  | I8    | 348  | ASP  | CA-C-N     | 5.16  | 124.95      | 119.28   |
| 22  | I8    | 348  | ASP  | C-N-CA     | 5.16  | 124.95      | 119.28   |
| 2   | M     | 449  | PHE  | CA-C-N     | -5.15 | 113.34      | 122.26   |
| 2   | M     | 449  | PHE  | C-N-CA     | -5.15 | 113.34      | 122.26   |
| 2   | M16   | 354  | ASP  | O-C-N      | -5.15 | 115.73      | 122.59   |
| 10  | C24   | 578  | LEU  | CA-C-N     | 5.15  | 128.14      | 120.31   |
| 10  | C24   | 578  | LEU  | C-N-CA     | 5.15  | 128.14      | 120.31   |
| 1   | R16   | 801  | PHE  | CB-CA-C    | -5.15 | 101.92      | 110.68   |
| 18  | B8    | 1714 | MET  | O-C-N      | -5.15 | 116.01      | 122.35   |
| 8   | L8    | 526  | GLN  | OE1-CD-NE2 | -5.15 | 117.45      | 122.60   |
| 10  | C     | 304  | GLY  | CA-C-N     | 5.15  | 129.32      | 120.72   |
| 10  | C     | 304  | GLY  | C-N-CA     | 5.15  | 129.32      | 120.72   |
| 22  | I16   | 129  | GLU  | O-C-N      | -5.15 | 116.77      | 122.07   |
| 15  | J     | 719  | LYS  | CA-C-N     | 5.15  | 127.73      | 120.42   |
| 15  | J     | 719  | LYS  | C-N-CA     | 5.15  | 127.73      | 120.42   |
| 10  | C32   | 578  | LEU  | CA-C-N     | 5.15  | 128.14      | 120.31   |
| 10  | C32   | 578  | LEU  | C-N-CA     | 5.15  | 128.14      | 120.31   |
| 10  | C32   | 1063 | PRO  | CA-C-N     | -5.15 | 111.70      | 121.54   |
| 10  | C32   | 1063 | PRO  | C-N-CA     | -5.15 | 111.70      | 121.54   |
| 2   | M16   | 449  | PHE  | CA-C-N     | -5.15 | 113.35      | 122.26   |
| 2   | M16   | 449  | PHE  | C-N-CA     | -5.15 | 113.35      | 122.26   |
| 7   | Q8    | 303  | LEU  | CA-C-N     | -5.15 | 114.48      | 119.78   |
| 7   | Q8    | 303  | LEU  | C-N-CA     | -5.15 | 114.48      | 119.78   |
| 6   | O16   | 120  | LYS  | CA-C-N     | -5.15 | 113.00      | 121.80   |
| 6   | O16   | 120  | LYS  | C-N-CA     | -5.15 | 113.00      | 121.80   |
| 9   | K     | 748  | THR  | O-C-N      | -5.15 | 115.14      | 122.96   |
| 10  | C16   | 1080 | SER  | CA-C-N     | 5.15  | 131.37      | 121.54   |
| 10  | C16   | 1080 | SER  | C-N-CA     | 5.15  | 131.37      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B     | 1714 | MET  | O-C-N      | -5.15 | 116.02      | 122.35   |
| 20  | E     | 200  | LEU  | CA-C-N     | -5.15 | 114.84      | 122.41   |
| 20  | E     | 200  | LEU  | C-N-CA     | -5.15 | 114.84      | 122.41   |
| 8   | L16   | 526  | GLN  | OE1-CD-NE2 | -5.15 | 117.45      | 122.60   |
| 18  | B     | 1098 | MET  | O-C-N      | 5.15  | 128.02      | 122.15   |
| 18  | B8    | 378  | ASN  | O-C-N      | 5.14  | 129.27      | 122.43   |
| 5   | P8    | 63   | ASP  | O-C-N      | -5.14 | 115.59      | 122.43   |
| 7   | Q8    | 223  | GLN  | O-C-N      | -5.14 | 115.75      | 122.59   |
| 5   | P16   | 63   | ASP  | O-C-N      | -5.14 | 115.59      | 122.43   |
| 22  | I24   | 129  | GLU  | O-C-N      | -5.14 | 116.78      | 122.07   |
| 9   | K     | 1120 | GLY  | O-C-N      | -5.14 | 116.02      | 122.70   |
| 10  | C24   | 1119 | GLU  | O-C-N      | 5.14  | 127.57      | 122.12   |
| 21  | H8    | 325  | PRO  | O-C-N      | 5.14  | 129.12      | 122.85   |
| 21  | H24   | 325  | PRO  | O-C-N      | 5.14  | 129.12      | 122.85   |
| 10  | C32   | 985  | LYS  | O-C-N      | 5.14  | 129.07      | 122.39   |
| 10  | C16   | 725  | LEU  | CA-C-N     | -5.14 | 113.40      | 120.28   |
| 10  | C16   | 725  | LEU  | C-N-CA     | -5.14 | 113.40      | 120.28   |
| 23  | J24   | 614  | ASP  | O-C-N      | 5.14  | 127.56      | 122.12   |
| 9   | K8    | 748  | THR  | O-C-N      | -5.13 | 115.16      | 122.96   |
| 10  | C32   | 1657 | SER  | CA-C-N     | 5.13  | 131.34      | 121.54   |
| 10  | C32   | 1657 | SER  | C-N-CA     | 5.13  | 131.34      | 121.54   |
| 10  | C24   | 335  | ASP  | O-C-N      | -5.13 | 115.76      | 122.59   |
| 11  | A40   | 558  | SER  | O-C-N      | -5.13 | 116.71      | 122.97   |
| 10  | C8    | 931  | PRO  | O-C-N      | -5.13 | 115.36      | 122.24   |
| 2   | M8    | 449  | PHE  | CA-C-N     | -5.13 | 113.38      | 122.26   |
| 2   | M8    | 449  | PHE  | C-N-CA     | -5.13 | 113.38      | 122.26   |
| 10  | C     | 1716 | LYS  | O-C-N      | 5.13  | 128.00      | 122.15   |
| 9   | K     | 604  | SER  | CA-C-N     | 5.13  | 127.42      | 120.44   |
| 9   | K     | 604  | SER  | C-N-CA     | 5.13  | 127.42      | 120.44   |
| 10  | C     | 1119 | GLU  | O-C-N      | 5.13  | 127.56      | 122.12   |
| 10  | C16   | 304  | GLY  | CA-C-N     | 5.13  | 129.28      | 120.72   |
| 10  | C16   | 304  | GLY  | C-N-CA     | 5.13  | 129.28      | 120.72   |
| 10  | C16   | 1063 | PRO  | CA-C-N     | -5.13 | 111.75      | 121.54   |
| 10  | C16   | 1063 | PRO  | C-N-CA     | -5.13 | 111.75      | 121.54   |
| 11  | A24   | 558  | SER  | O-C-N      | -5.13 | 116.71      | 122.97   |
| 10  | C24   | 1042 | GLU  | O-C-N      | 5.13  | 127.56      | 122.12   |
| 10  | C     | 578  | LEU  | CA-C-N     | 5.13  | 128.10      | 120.31   |
| 10  | C     | 578  | LEU  | C-N-CA     | 5.13  | 128.10      | 120.31   |
| 10  | C8    | 169  | GLN  | O-C-N      | 5.13  | 127.56      | 122.12   |
| 10  | C8    | 1514 | ASN  | O-C-N      | 5.13  | 128.58      | 122.27   |
| 19  | 4     | 375  | ASP  | CA-C-N     | 5.13  | 127.66      | 120.28   |
| 19  | 4     | 375  | ASP  | C-N-CA     | 5.13  | 127.66      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 7   | Q8    | 269  | VAL  | O-C-N      | -5.13 | 117.08      | 122.67   |
| 7   | Q16   | 303  | LEU  | CA-C-N     | -5.13 | 114.50      | 119.78   |
| 7   | Q16   | 303  | LEU  | C-N-CA     | -5.13 | 114.50      | 119.78   |
| 9   | K8    | 853  | ALA  | O-C-N      | -5.13 | 115.77      | 122.59   |
| 18  | B     | 504  | PRO  | O-C-N      | -5.13 | 115.72      | 122.64   |
| 22  | I     | 129  | GLU  | O-C-N      | -5.13 | 116.79      | 122.07   |
| 24  | D16   | 320  | PRO  | N-CA-CB    | 5.13  | 107.81      | 103.35   |
| 9   | K     | 853  | ALA  | O-C-N      | -5.12 | 115.77      | 122.59   |
| 10  | C8    | 578  | LEU  | CA-C-N     | 5.12  | 128.10      | 120.31   |
| 10  | C8    | 578  | LEU  | C-N-CA     | 5.12  | 128.10      | 120.31   |
| 18  | B8    | 969  | ASP  | O-C-N      | -5.12 | 116.63      | 122.93   |
| 2   | M     | 328  | THR  | CA-C-N     | -5.12 | 113.42      | 120.28   |
| 2   | M     | 328  | THR  | C-N-CA     | -5.12 | 113.42      | 120.28   |
| 7   | Q     | 223  | GLN  | O-C-N      | -5.12 | 115.77      | 122.59   |
| 10  | C16   | 1657 | SER  | CA-C-N     | 5.12  | 131.33      | 121.54   |
| 10  | C16   | 1657 | SER  | C-N-CA     | 5.12  | 131.33      | 121.54   |
| 11  | A16   | 558  | SER  | O-C-N      | -5.12 | 116.72      | 122.97   |
| 18  | B     | 1666 | PRO  | CA-C-N     | 5.12  | 128.12      | 120.95   |
| 18  | B     | 1666 | PRO  | C-N-CA     | 5.12  | 128.12      | 120.95   |
| 24  | D8    | 320  | PRO  | N-CA-CB    | 5.12  | 107.81      | 103.35   |
| 18  | B8    | 1800 | ARG  | CA-C-N     | -5.12 | 111.37      | 121.41   |
| 18  | B8    | 1800 | ARG  | C-N-CA     | -5.12 | 111.37      | 121.41   |
| 18  | B8    | 1792 | SER  | O-C-N      | -5.12 | 115.78      | 122.59   |
| 18  | B8    | 1801 | GLY  | CA-C-N     | 5.12  | 131.32      | 121.54   |
| 18  | B8    | 1801 | GLY  | C-N-CA     | 5.12  | 131.32      | 121.54   |
| 10  | C8    | 1331 | CYS  | O-C-N      | -5.12 | 115.58      | 122.23   |
| 22  | I8    | 363  | ALA  | O-C-N      | 5.12  | 127.55      | 122.12   |
| 1   | R8    | 801  | PHE  | CB-CA-C    | -5.12 | 101.98      | 110.68   |
| 18  | B     | 134  | GLN  | O-C-N      | 5.12  | 127.98      | 122.15   |
| 18  | B     | 1141 | ILE  | O-C-N      | 5.12  | 127.10      | 121.83   |
| 18  | B8    | 475  | GLU  | O-C-N      | -5.12 | 116.17      | 122.82   |
| 10  | C32   | 1119 | GLU  | O-C-N      | 5.12  | 127.54      | 122.12   |
| 5   | P16   | 331  | HIS  | CA-C-N     | 5.11  | 127.55      | 120.29   |
| 5   | P16   | 331  | HIS  | C-N-CA     | 5.11  | 127.55      | 120.29   |
| 9   | K8    | 1257 | ALA  | CA-C-N     | 5.11  | 125.66      | 119.98   |
| 9   | K8    | 1257 | ALA  | C-N-CA     | 5.11  | 125.66      | 119.98   |
| 9   | K16   | 924  | GLN  | OE1-CD-NE2 | -5.11 | 117.49      | 122.60   |
| 10  | C24   | 169  | GLN  | O-C-N      | 5.11  | 127.54      | 122.12   |
| 14  | W     | 610  | PRO  | O-C-N      | -5.11 | 116.61      | 122.85   |
| 10  | C     | 880  | GLU  | O-C-N      | 5.11  | 129.67      | 122.41   |
| 10  | C     | 1514 | ASN  | O-C-N      | 5.11  | 128.56      | 122.27   |
| 18  | B     | 1801 | GLY  | CA-C-N     | 5.11  | 131.31      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B     | 1801 | GLY  | C-N-CA     | 5.11  | 131.31      | 121.54   |
| 22  | I     | 351  | LEU  | O-C-N      | 5.11  | 127.54      | 122.12   |
| 14  | W     | 637  | LYS  | CA-C-N     | 5.11  | 127.00      | 120.56   |
| 14  | W     | 637  | LYS  | C-N-CA     | 5.11  | 127.00      | 120.56   |
| 10  | C     | 1063 | PRO  | CA-C-N     | -5.11 | 111.78      | 121.54   |
| 10  | C     | 1063 | PRO  | C-N-CA     | -5.11 | 111.78      | 121.54   |
| 1   | R     | 1459 | ARG  | O-C-N      | -5.11 | 117.49      | 123.27   |
| 1   | R8    | 1386 | MET  | O-C-N      | 5.11  | 128.37      | 122.19   |
| 2   | M8    | 288  | ILE  | O-C-N      | 5.11  | 126.83      | 121.87   |
| 10  | C16   | 1383 | GLY  | O-C-N      | -5.11 | 117.28      | 122.19   |
| 10  | C     | 725  | LEU  | CA-C-N     | -5.11 | 113.43      | 120.28   |
| 10  | C     | 725  | LEU  | C-N-CA     | -5.11 | 113.43      | 120.28   |
| 10  | C     | 1290 | HIS  | CA-C-N     | -5.11 | 113.70      | 121.31   |
| 10  | C     | 1290 | HIS  | C-N-CA     | -5.11 | 113.70      | 121.31   |
| 18  | B8    | 1141 | ILE  | O-C-N      | 5.11  | 127.09      | 121.83   |
| 22  | I24   | 363  | ALA  | O-C-N      | 5.11  | 127.54      | 122.12   |
| 7   | Q     | 269  | VAL  | O-C-N      | -5.11 | 117.10      | 122.67   |
| 7   | Q8    | 308  | CYS  | CA-C-N     | -5.11 | 114.19      | 122.36   |
| 7   | Q8    | 308  | CYS  | C-N-CA     | -5.11 | 114.19      | 122.36   |
| 18  | B     | 1877 | ALA  | O-C-N      | 5.11  | 127.53      | 122.12   |
| 23  | J32   | 735  | LYS  | CA-C-N     | -5.11 | 109.57      | 121.52   |
| 23  | J32   | 735  | LYS  | C-N-CA     | -5.11 | 109.57      | 121.52   |
| 7   | Q     | 308  | CYS  | CA-C-N     | -5.11 | 114.19      | 122.36   |
| 7   | Q     | 308  | CYS  | C-N-CA     | -5.11 | 114.19      | 122.36   |
| 10  | C24   | 1514 | ASN  | O-C-N      | 5.11  | 128.55      | 122.27   |
| 18  | B     | 969  | ASP  | O-C-N      | -5.11 | 116.65      | 122.93   |
| 20  | E8    | 200  | LEU  | CA-C-N     | -5.11 | 114.90      | 122.41   |
| 20  | E8    | 200  | LEU  | C-N-CA     | -5.11 | 114.90      | 122.41   |
| 10  | C24   | 304  | GLY  | CA-C-N     | 5.10  | 129.24      | 120.72   |
| 10  | C24   | 304  | GLY  | C-N-CA     | 5.10  | 129.24      | 120.72   |
| 18  | B     | 1800 | ARG  | CA-C-N     | -5.10 | 111.41      | 121.41   |
| 18  | B     | 1800 | ARG  | C-N-CA     | -5.10 | 111.41      | 121.41   |
| 9   | K     | 1257 | ALA  | CA-C-N     | 5.10  | 125.64      | 119.98   |
| 9   | K     | 1257 | ALA  | C-N-CA     | 5.10  | 125.64      | 119.98   |
| 10  | C24   | 985  | LYS  | O-C-N      | 5.10  | 129.02      | 122.39   |
| 10  | C     | 662  | LEU  | O-C-N      | 5.10  | 127.53      | 122.12   |
| 1   | R16   | 1459 | ARG  | O-C-N      | -5.10 | 117.50      | 123.27   |
| 18  | B     | 1792 | SER  | O-C-N      | -5.10 | 115.81      | 122.59   |
| 10  | C32   | 662  | LEU  | O-C-N      | 5.10  | 127.53      | 122.12   |
| 2   | M8    | 328  | THR  | CA-C-N     | -5.10 | 113.39      | 120.38   |
| 2   | M8    | 328  | THR  | C-N-CA     | -5.10 | 113.39      | 120.38   |
| 4   | T8    | 226  | GLN  | OE1-CD-NE2 | -5.10 | 117.50      | 122.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10  | C16   | 1042 | GLU  | O-C-N      | 5.10  | 127.53      | 122.12   |
| 10  | C32   | 1514 | ASN  | O-C-N      | 5.10  | 128.54      | 122.27   |
| 10  | C24   | 1687 | GLU  | O-C-N      | 5.10  | 127.52      | 122.12   |
| 18  | B8    | 1877 | ALA  | O-C-N      | 5.10  | 127.52      | 122.12   |
| 23  | J8    | 735  | LYS  | CA-C-N     | -5.10 | 109.59      | 121.52   |
| 23  | J8    | 735  | LYS  | C-N-CA     | -5.10 | 109.59      | 121.52   |
| 10  | C24   | 1063 | PRO  | CA-C-N     | -5.10 | 111.81      | 121.54   |
| 10  | C24   | 1063 | PRO  | C-N-CA     | -5.10 | 111.81      | 121.54   |
| 18  | B     | 378  | ASN  | O-C-N      | 5.10  | 129.21      | 122.43   |
| 23  | J24   | 735  | LYS  | CA-C-N     | -5.10 | 109.60      | 121.52   |
| 23  | J24   | 735  | LYS  | C-N-CA     | -5.10 | 109.60      | 121.52   |
| 22  | I16   | 351  | LEU  | O-C-N      | 5.10  | 127.52      | 122.12   |
| 5   | P8    | 24   | VAL  | O-C-N      | -5.09 | 117.15      | 122.81   |
| 7   | Q16   | 223  | GLN  | O-C-N      | -5.09 | 115.81      | 122.59   |
| 9   | K8    | 746  | ARG  | O-C-N      | 5.09  | 128.18      | 122.22   |
| 9   | K16   | 998  | GLN  | OE1-CD-NE2 | -5.09 | 117.50      | 122.60   |
| 10  | C     | 1042 | GLU  | O-C-N      | 5.09  | 127.52      | 122.12   |
| 10  | C8    | 898  | GLN  | O-C-N      | 5.09  | 127.52      | 122.12   |
| 23  | J16   | 735  | LYS  | CA-C-N     | -5.09 | 109.60      | 121.52   |
| 23  | J16   | 735  | LYS  | C-N-CA     | -5.09 | 109.60      | 121.52   |
| 10  | C32   | 169  | GLN  | O-C-N      | 5.09  | 127.52      | 122.12   |
| 9   | K8    | 1190 | GLU  | O-C-N      | -5.09 | 116.23      | 122.34   |
| 8   | L     | 526  | GLN  | OE1-CD-NE2 | -5.09 | 117.51      | 122.60   |
| 9   | K     | 746  | ARG  | O-C-N      | 5.09  | 128.18      | 122.22   |
| 10  | C     | 335  | ASP  | O-C-N      | -5.09 | 115.82      | 122.59   |
| 10  | C8    | 304  | GLY  | CA-C-N     | 5.09  | 129.22      | 120.72   |
| 10  | C8    | 304  | GLY  | C-N-CA     | 5.09  | 129.22      | 120.72   |
| 18  | B     | 1100 | LEU  | O-C-N      | 5.09  | 127.52      | 122.12   |
| 22  | I8    | 129  | GLU  | O-C-N      | -5.09 | 116.83      | 122.07   |
| 10  | C32   | 1290 | HIS  | CA-C-N     | -5.09 | 113.72      | 121.31   |
| 10  | C32   | 1290 | HIS  | C-N-CA     | -5.09 | 113.72      | 121.31   |
| 1   | R8    | 1459 | ARG  | O-C-N      | -5.09 | 117.52      | 123.27   |
| 9   | K8    | 604  | SER  | CA-C-N     | 5.09  | 127.36      | 120.44   |
| 9   | K8    | 604  | SER  | C-N-CA     | 5.09  | 127.36      | 120.44   |
| 10  | C16   | 985  | LYS  | O-C-N      | 5.09  | 129.00      | 122.39   |
| 10  | C16   | 1290 | HIS  | CA-C-N     | -5.09 | 113.73      | 121.31   |
| 10  | C16   | 1290 | HIS  | C-N-CA     | -5.09 | 113.73      | 121.31   |
| 24  | D40   | 320  | PRO  | N-CA-CB    | 5.09  | 107.78      | 103.35   |
| 10  | C8    | 662  | LEU  | O-C-N      | 5.09  | 127.51      | 122.12   |
| 18  | B8    | 1549 | GLN  | O-C-N      | 5.09  | 129.63      | 122.41   |
| 21  | H8    | 295  | GLY  | O-C-N      | 5.09  | 128.07      | 122.27   |
| 22  | I8    | 113  | HIS  | CA-C-N     | 5.09  | 125.37      | 119.47   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | I8    | 113  | HIS  | C-N-CA  | 5.09  | 125.37      | 119.47   |
| 21  | H16   | 325  | PRO  | O-C-N   | 5.09  | 129.06      | 122.85   |
| 2   | M8    | 538  | LEU  | O-C-N   | 5.09  | 127.51      | 122.12   |
| 9   | K8    | 1068 | GLN  | CA-C-N  | -5.09 | 113.48      | 119.84   |
| 9   | K8    | 1068 | GLN  | C-N-CA  | -5.09 | 113.48      | 119.84   |
| 18  | B8    | 1677 | ARG  | O-C-N   | -5.09 | 116.73      | 122.12   |
| 9   | K     | 1190 | GLU  | O-C-N   | -5.08 | 116.24      | 122.34   |
| 21  | H24   | 164  | ALA  | O-C-N   | -5.08 | 116.27      | 122.22   |
| 2   | M     | 846  | LEU  | O-C-N   | 5.08  | 127.94      | 122.15   |
| 9   | K     | 1279 | GLU  | CA-C-N  | -5.08 | 113.73      | 121.66   |
| 9   | K     | 1279 | GLU  | C-N-CA  | -5.08 | 113.73      | 121.66   |
| 9   | K8    | 1120 | GLY  | O-C-N   | -5.08 | 116.09      | 122.70   |
| 9   | K8    | 1279 | GLU  | CA-C-N  | -5.08 | 113.73      | 121.66   |
| 9   | K8    | 1279 | GLU  | C-N-CA  | -5.08 | 113.73      | 121.66   |
| 10  | C16   | 1334 | MET  | CA-C-N  | 5.08  | 129.73      | 123.12   |
| 10  | C16   | 1334 | MET  | C-N-CA  | 5.08  | 129.73      | 123.12   |
| 10  | C24   | 980  | ASP  | O-C-N   | 5.08  | 127.51      | 122.12   |
| 10  | C24   | 1331 | CYS  | O-C-N   | -5.08 | 115.62      | 122.23   |
| 10  | C8    | 1042 | GLU  | O-C-N   | 5.08  | 127.51      | 122.12   |
| 22  | I     | 113  | HIS  | CA-C-N  | 5.08  | 125.37      | 119.47   |
| 22  | I     | 113  | HIS  | C-N-CA  | 5.08  | 125.37      | 119.47   |
| 10  | C24   | 1625 | SER  | CA-C-N  | 5.08  | 131.25      | 121.54   |
| 10  | C24   | 1625 | SER  | C-N-CA  | 5.08  | 131.25      | 121.54   |
| 18  | B     | 1681 | GLN  | O-C-N   | -5.08 | 115.83      | 122.59   |
| 10  | C32   | 335  | ASP  | O-C-N   | -5.08 | 115.83      | 122.59   |
| 9   | K8    | 1235 | GLU  | CA-C-N  | 5.08  | 129.75      | 121.83   |
| 9   | K8    | 1235 | GLU  | C-N-CA  | 5.08  | 129.75      | 121.83   |
| 10  | C24   | 880  | GLU  | O-C-N   | 5.08  | 129.62      | 122.41   |
| 18  | B8    | 1798 | VAL  | CA-C-N  | -5.08 | 112.83      | 121.97   |
| 18  | B8    | 1798 | VAL  | C-N-CA  | -5.08 | 112.83      | 121.97   |
| 22  | I8    | 351  | LEU  | O-C-N   | 5.08  | 127.50      | 122.12   |
| 10  | C24   | 1657 | SER  | CA-C-N  | 5.08  | 131.24      | 121.54   |
| 10  | C24   | 1657 | SER  | C-N-CA  | 5.08  | 131.24      | 121.54   |
| 20  | E8    | 518  | GLN  | O-C-N   | 5.08  | 128.82      | 122.22   |
| 21  | H16   | 164  | ALA  | O-C-N   | -5.08 | 116.28      | 122.22   |
| 10  | C     | 1115 | ASP  | O-C-N   | 5.08  | 127.30      | 122.07   |
| 10  | C8    | 672  | ASP  | CA-C-N  | 5.08  | 129.25      | 122.95   |
| 10  | C8    | 672  | ASP  | C-N-CA  | 5.08  | 129.25      | 122.95   |
| 24  | D     | 320  | PRO  | N-CA-CB | 5.08  | 107.77      | 103.35   |
| 1   | R8    | 1144 | CYS  | CA-C-N  | -5.08 | 113.98      | 123.01   |
| 1   | R8    | 1144 | CYS  | C-N-CA  | -5.08 | 113.98      | 123.01   |
| 5   | P8    | 331  | HIS  | CA-C-N  | 5.08  | 127.50      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | P8    | 331  | HIS  | C-N-CA     | 5.08  | 127.50      | 120.29   |
| 4   | T16   | 126  | GLN  | OE1-CD-NE2 | -5.07 | 117.53      | 122.60   |
| 9   | K16   | 1021 | SER  | CA-C-N     | 5.07  | 127.59      | 120.28   |
| 9   | K16   | 1021 | SER  | C-N-CA     | 5.07  | 127.59      | 120.28   |
| 18  | B     | 1549 | GLN  | O-C-N      | 5.07  | 129.61      | 122.41   |
| 22  | I16   | 113  | HIS  | CA-C-N     | 5.07  | 125.36      | 119.47   |
| 22  | I16   | 113  | HIS  | C-N-CA     | 5.07  | 125.36      | 119.47   |
| 10  | C32   | 725  | LEU  | CA-C-N     | -5.07 | 113.48      | 120.28   |
| 10  | C32   | 725  | LEU  | C-N-CA     | -5.07 | 113.48      | 120.28   |
| 9   | K     | 1230 | LEU  | O-C-N      | 5.07  | 125.33      | 121.27   |
| 10  | C24   | 1290 | HIS  | CA-C-N     | -5.07 | 113.75      | 121.31   |
| 10  | C24   | 1290 | HIS  | C-N-CA     | -5.07 | 113.75      | 121.31   |
| 10  | C16   | 335  | ASP  | O-C-N      | -5.07 | 115.84      | 122.59   |
| 10  | C16   | 770  | SER  | CA-C-N     | -5.07 | 114.85      | 122.81   |
| 10  | C16   | 770  | SER  | C-N-CA     | -5.07 | 114.85      | 122.81   |
| 10  | C     | 1331 | CYS  | O-C-N      | -5.07 | 115.64      | 122.23   |
| 10  | C8    | 673  | VAL  | CA-C-N     | 5.07  | 129.64      | 122.24   |
| 10  | C8    | 673  | VAL  | C-N-CA     | 5.07  | 129.64      | 122.24   |
| 17  | F16   | 55   | PRO  | O-C-N      | 5.07  | 127.44      | 121.46   |
| 23  | J32   | 729  | ARG  | CA-C-N     | -5.07 | 113.49      | 120.28   |
| 23  | J32   | 729  | ARG  | C-N-CA     | -5.07 | 113.49      | 120.28   |
| 9   | K     | 1283 | PRO  | CA-C-N     | -5.07 | 112.17      | 122.31   |
| 9   | K     | 1283 | PRO  | C-N-CA     | -5.07 | 112.17      | 122.31   |
| 18  | B     | 1009 | ALA  | O-C-N      | -5.07 | 116.75      | 122.12   |
| 18  | B8    | 1666 | PRO  | CA-C-N     | 5.07  | 128.04      | 120.95   |
| 18  | B8    | 1666 | PRO  | C-N-CA     | 5.07  | 128.04      | 120.95   |
| 22  | I16   | 363  | ALA  | O-C-N      | 5.07  | 127.49      | 122.12   |
| 23  | J16   | 729  | ARG  | CA-C-N     | -5.07 | 113.49      | 120.28   |
| 23  | J16   | 729  | ARG  | C-N-CA     | -5.07 | 113.49      | 120.28   |
| 4   | T8    | 75   | HIS  | N-CA-C     | 5.07  | 117.53      | 111.71   |
| 10  | C24   | 725  | LEU  | CA-C-N     | -5.07 | 113.49      | 120.28   |
| 10  | C24   | 725  | LEU  | C-N-CA     | -5.07 | 113.49      | 120.28   |
| 17  | F24   | 55   | PRO  | O-C-N      | 5.07  | 127.44      | 121.46   |
| 18  | B     | 849  | SER  | O-C-N      | -5.07 | 115.47      | 122.46   |
| 18  | B8    | 1100 | LEU  | O-C-N      | 5.07  | 127.49      | 122.12   |
| 17  | F     | 55   | PRO  | O-C-N      | 5.06  | 127.44      | 121.46   |
| 21  | H     | 295  | GLY  | O-C-N      | 5.06  | 128.04      | 122.27   |
| 24  | D8    | 1069 | GLY  | CA-C-N     | 5.06  | 127.96      | 120.82   |
| 24  | D8    | 1069 | GLY  | C-N-CA     | 5.06  | 127.96      | 120.82   |
| 1   | R16   | 1386 | MET  | O-C-N      | 5.06  | 128.31      | 122.19   |
| 5   | P8    | 59   | LEU  | CA-C-N     | 5.06  | 132.42      | 121.64   |
| 5   | P8    | 59   | LEU  | C-N-CA     | 5.06  | 132.42      | 121.64   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 1235 | GLU  | CA-C-N | 5.06  | 129.73      | 121.83   |
| 9   | K     | 1235 | GLU  | C-N-CA | 5.06  | 129.73      | 121.83   |
| 10  | C     | 636  | VAL  | O-C-N  | -5.06 | 116.84      | 122.66   |
| 18  | B     | 1677 | ARG  | O-C-N  | -5.06 | 116.75      | 122.12   |
| 24  | D16   | 1069 | GLY  | CA-C-N | 5.06  | 127.96      | 120.82   |
| 24  | D16   | 1069 | GLY  | C-N-CA | 5.06  | 127.96      | 120.82   |
| 10  | C32   | 1664 | SER  | O-C-N  | -5.06 | 115.86      | 122.59   |
| 10  | C8    | 980  | ASP  | O-C-N  | 5.06  | 127.48      | 122.12   |
| 2   | M16   | 553  | GLY  | O-C-N  | -5.06 | 117.33      | 122.19   |
| 5   | P16   | 59   | LEU  | CA-C-N | 5.06  | 132.42      | 121.64   |
| 5   | P16   | 59   | LEU  | C-N-CA | 5.06  | 132.42      | 121.64   |
| 9   | K8    | 1230 | LEU  | O-C-N  | 5.06  | 125.32      | 121.27   |
| 10  | C24   | 1334 | MET  | CA-C-N | 5.06  | 129.70      | 123.12   |
| 10  | C24   | 1334 | MET  | C-N-CA | 5.06  | 129.70      | 123.12   |
| 18  | B     | 1127 | PRO  | CA-C-N | 5.06  | 126.17      | 119.84   |
| 18  | B     | 1127 | PRO  | C-N-CA | 5.06  | 126.17      | 119.84   |
| 10  | C32   | 429  | SER  | O-C-N  | -5.06 | 116.24      | 122.11   |
| 1   | R     | 888  | ASP  | CA-C-N | 5.06  | 128.77      | 120.63   |
| 1   | R     | 888  | ASP  | C-N-CA | 5.06  | 128.77      | 120.63   |
| 2   | M8    | 846  | LEU  | O-C-N  | 5.06  | 127.92      | 122.15   |
| 9   | K     | 1218 | ARG  | O-C-N  | -5.06 | 116.28      | 123.01   |
| 9   | K8    | 1283 | PRO  | CA-C-N | -5.06 | 112.20      | 122.31   |
| 9   | K8    | 1283 | PRO  | C-N-CA | -5.06 | 112.20      | 122.31   |
| 18  | B8    | 1681 | GLN  | O-C-N  | -5.06 | 115.86      | 122.59   |
| 9   | K8    | 897  | LEU  | O-C-N  | 5.05  | 127.91      | 122.15   |
| 21  | H8    | 164  | ALA  | O-C-N  | -5.05 | 116.31      | 122.22   |
| 24  | D32   | 759  | TYR  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 10  | C32   | 980  | ASP  | O-C-N  | 5.05  | 127.48      | 122.12   |
| 5   | P     | 24   | VAL  | O-C-N  | -5.05 | 117.20      | 122.81   |
| 5   | P     | 59   | LEU  | CA-C-N | 5.05  | 132.40      | 121.64   |
| 5   | P     | 59   | LEU  | C-N-CA | 5.05  | 132.40      | 121.64   |
| 5   | P     | 331  | HIS  | CA-C-N | 5.05  | 127.46      | 120.29   |
| 5   | P     | 331  | HIS  | C-N-CA | 5.05  | 127.46      | 120.29   |
| 10  | C16   | 1115 | ASP  | O-C-N  | 5.05  | 127.27      | 122.07   |
| 23  | J24   | 729  | ARG  | CA-C-N | -5.05 | 113.51      | 120.28   |
| 23  | J24   | 729  | ARG  | C-N-CA | -5.05 | 113.51      | 120.28   |
| 10  | C16   | 880  | GLU  | O-C-N  | 5.05  | 129.58      | 122.41   |
| 10  | C8    | 1332 | GLN  | O-C-N  | -5.05 | 116.06      | 122.27   |
| 18  | B     | 475  | GLU  | O-C-N  | -5.05 | 116.25      | 122.82   |
| 20  | E     | 518  | GLN  | O-C-N  | 5.05  | 128.78      | 122.22   |
| 22  | I     | 363  | ALA  | O-C-N  | 5.05  | 127.47      | 122.12   |
| 10  | C32   | 1698 | HIS  | O-C-N  | 5.05  | 127.91      | 122.15   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | M16   | 538  | LEU  | O-C-N    | 5.05  | 127.47      | 122.12   |
| 1   | R16   | 1144 | CYS  | CA-C-N   | -5.05 | 114.03      | 123.01   |
| 1   | R16   | 1144 | CYS  | C-N-CA   | -5.05 | 114.03      | 123.01   |
| 22  | I     | 345  | GLU  | O-C-N    | -5.05 | 116.88      | 122.93   |
| 10  | C32   | 880  | GLU  | O-C-N    | 5.05  | 129.58      | 122.41   |
| 10  | C32   | 1383 | GLY  | O-C-N    | -5.05 | 117.35      | 122.19   |
| 4   | T16   | 75   | HIS  | N-CA-C   | 5.04  | 117.51      | 111.71   |
| 18  | B8    | 1127 | PRO  | CA-C-N   | 5.04  | 126.15      | 119.84   |
| 18  | B8    | 1127 | PRO  | C-N-CA   | 5.04  | 126.15      | 119.84   |
| 10  | C     | 306  | ASP  | CA-C-N   | 5.04  | 124.35      | 118.85   |
| 10  | C     | 306  | ASP  | C-N-CA   | 5.04  | 124.35      | 118.85   |
| 18  | B8    | 849  | SER  | O-C-N    | -5.04 | 115.50      | 122.46   |
| 24  | D     | 450  | GLY  | CA-C-N   | 5.04  | 131.17      | 121.54   |
| 24  | D     | 450  | GLY  | C-N-CA   | 5.04  | 131.17      | 121.54   |
| 2   | M16   | 460  | TYR  | O-C-N    | 5.04  | 127.90      | 122.15   |
| 10  | C     | 672  | ASP  | CA-C-N   | 5.04  | 129.20      | 122.95   |
| 10  | C     | 672  | ASP  | C-N-CA   | 5.04  | 129.20      | 122.95   |
| 10  | C     | 1773 | ARG  | O-C-N    | -5.04 | 115.89      | 122.59   |
| 18  | B8    | 1009 | ALA  | O-C-N    | -5.04 | 116.78      | 122.12   |
| 21  | H16   | 295  | GLY  | O-C-N    | 5.04  | 128.02      | 122.27   |
| 9   | K     | 1068 | GLN  | CA-C-N   | -5.04 | 113.54      | 119.84   |
| 9   | K     | 1068 | GLN  | C-N-CA   | -5.04 | 113.54      | 119.84   |
| 18  | B     | 1798 | VAL  | CA-C-N   | -5.04 | 112.90      | 121.97   |
| 18  | B     | 1798 | VAL  | C-N-CA   | -5.04 | 112.90      | 121.97   |
| 24  | D     | 1069 | GLY  | CA-C-N   | 5.04  | 127.93      | 120.82   |
| 24  | D     | 1069 | GLY  | C-N-CA   | 5.04  | 127.93      | 120.82   |
| 24  | D24   | 320  | PRO  | N-CA-CB  | 5.04  | 107.73      | 103.35   |
| 24  | D40   | 1069 | GLY  | CA-C-N   | 5.04  | 127.93      | 120.82   |
| 24  | D40   | 1069 | GLY  | C-N-CA   | 5.04  | 127.93      | 120.82   |
| 2   | M16   | 846  | LEU  | O-C-N    | 5.04  | 127.89      | 122.15   |
| 4   | T     | 508  | ARG  | CD-NE-CZ | 5.04  | 131.45      | 124.40   |
| 10  | C24   | 673  | VAL  | CA-C-N   | 5.04  | 129.59      | 122.24   |
| 10  | C24   | 673  | VAL  | C-N-CA   | 5.04  | 129.59      | 122.24   |
| 10  | C8    | 880  | GLU  | O-C-N    | 5.04  | 129.56      | 122.41   |
| 24  | D     | 759  | TYR  | N-CA-C   | 5.04  | 121.53      | 110.80   |
| 10  | C32   | 770  | SER  | CA-C-N   | -5.04 | 114.90      | 122.81   |
| 10  | C32   | 770  | SER  | C-N-CA   | -5.04 | 114.90      | 122.81   |
| 20  | E8    | 435  | ALA  | CA-C-N   | -5.04 | 111.92      | 121.54   |
| 20  | E8    | 435  | ALA  | C-N-CA   | -5.04 | 111.92      | 121.54   |
| 2   | M     | 288  | ILE  | O-C-N    | 5.04  | 126.75      | 121.87   |
| 2   | M     | 460  | TYR  | O-C-N    | 5.04  | 127.89      | 122.15   |
| 2   | M8    | 553  | GLY  | O-C-N    | -5.04 | 117.36      | 122.19   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 18  | B     | 279  | LEU  | CA-C-N     | 5.04  | 129.51      | 122.36   |
| 18  | B     | 279  | LEU  | C-N-CA     | 5.04  | 129.51      | 122.36   |
| 21  | H24   | 295  | GLY  | O-C-N      | 5.04  | 128.01      | 122.27   |
| 10  | C32   | 1042 | GLU  | O-C-N      | 5.04  | 127.46      | 122.12   |
| 9   | K8    | 1218 | ARG  | O-C-N      | -5.03 | 116.31      | 123.01   |
| 10  | C24   | 770  | SER  | CA-C-N     | -5.03 | 114.91      | 122.81   |
| 10  | C24   | 770  | SER  | C-N-CA     | -5.03 | 114.91      | 122.81   |
| 10  | C     | 1664 | SER  | O-C-N      | -5.03 | 115.89      | 122.59   |
| 18  | B8    | 279  | LEU  | CA-C-N     | 5.03  | 129.51      | 122.36   |
| 18  | B8    | 279  | LEU  | C-N-CA     | 5.03  | 129.51      | 122.36   |
| 24  | D16   | 759  | TYR  | N-CA-C     | 5.03  | 121.52      | 110.80   |
| 10  | C32   | 1625 | SER  | CA-C-N     | 5.03  | 131.15      | 121.54   |
| 10  | C32   | 1625 | SER  | C-N-CA     | 5.03  | 131.15      | 121.54   |
| 9   | K8    | 926  | ILE  | CA-C-N     | 5.03  | 131.15      | 121.54   |
| 9   | K8    | 926  | ILE  | C-N-CA     | 5.03  | 131.15      | 121.54   |
| 18  | B     | 1747 | SER  | O-C-N      | -5.03 | 113.28      | 122.34   |
| 24  | D32   | 450  | GLY  | CA-C-N     | 5.03  | 131.15      | 121.54   |
| 24  | D32   | 450  | GLY  | C-N-CA     | 5.03  | 131.15      | 121.54   |
| 4   | T     | 226  | GLN  | OE1-CD-NE2 | -5.03 | 117.57      | 122.60   |
| 10  | C24   | 672  | ASP  | CA-C-N     | 5.03  | 129.19      | 122.95   |
| 10  | C24   | 672  | ASP  | C-N-CA     | 5.03  | 129.19      | 122.95   |
| 10  | C24   | 898  | GLN  | O-C-N      | 5.03  | 127.45      | 122.12   |
| 10  | C8    | 429  | SER  | O-C-N      | -5.03 | 116.28      | 122.11   |
| 24  | D     | 796  | ARG  | NE-CZ-NH2  | 5.03  | 123.73      | 119.20   |
| 10  | C32   | 1782 | SER  | O-C-N      | -5.03 | 116.62      | 122.96   |
| 1   | R     | 1484 | VAL  | O-C-N      | 5.03  | 127.01      | 121.83   |
| 7   | Q     | 303  | LEU  | CA-C-N     | -5.03 | 114.60      | 119.78   |
| 7   | Q     | 303  | LEU  | C-N-CA     | -5.03 | 114.60      | 119.78   |
| 6   | O16   | 51   | LYS  | CA-C-N     | -5.03 | 115.47      | 122.71   |
| 6   | O16   | 51   | LYS  | C-N-CA     | -5.03 | 115.47      | 122.71   |
| 7   | Q16   | 308  | CYS  | CA-C-N     | -5.03 | 114.31      | 122.36   |
| 7   | Q16   | 308  | CYS  | C-N-CA     | -5.03 | 114.31      | 122.36   |
| 10  | C8    | 922  | ALA  | CA-C-N     | -5.03 | 114.55      | 119.93   |
| 10  | C8    | 922  | ALA  | C-N-CA     | -5.03 | 114.55      | 119.93   |
| 21  | H     | 164  | ALA  | O-C-N      | -5.03 | 116.34      | 122.22   |
| 24  | D8    | 450  | GLY  | CA-C-N     | 5.03  | 131.14      | 121.54   |
| 24  | D8    | 450  | GLY  | C-N-CA     | 5.03  | 131.14      | 121.54   |
| 24  | D24   | 759  | TYR  | N-CA-C     | 5.03  | 121.51      | 110.80   |
| 10  | C32   | 1331 | CYS  | O-C-N      | -5.03 | 115.69      | 122.23   |
| 2   | M     | 756  | MET  | O-C-N      | -5.03 | 115.91      | 122.59   |
| 1   | R16   | 888  | ASP  | CA-C-N     | 5.03  | 128.72      | 120.63   |
| 1   | R16   | 888  | ASP  | C-N-CA     | 5.03  | 128.72      | 120.63   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9   | K     | 792  | LEU  | O-C-N  | 5.03  | 127.88      | 122.15   |
| 9   | K     | 926  | ILE  | CA-C-N | 5.03  | 131.14      | 121.54   |
| 9   | K     | 926  | ILE  | C-N-CA | 5.03  | 131.14      | 121.54   |
| 19  | 4     | 63   | GLY  | O-C-N  | -5.03 | 116.17      | 122.70   |
| 19  | 4     | 294  | SER  | CA-C-N | 5.03  | 131.14      | 121.54   |
| 19  | 4     | 294  | SER  | C-N-CA | 5.03  | 131.14      | 121.54   |
| 24  | D24   | 1069 | GLY  | CA-C-N | 5.03  | 127.91      | 120.82   |
| 24  | D24   | 1069 | GLY  | C-N-CA | 5.03  | 127.91      | 120.82   |
| 10  | C32   | 1508 | GLN  | O-C-N  | -5.03 | 115.91      | 122.59   |
| 1   | R     | 1216 | ILE  | O-C-N  | 5.02  | 126.74      | 121.87   |
| 24  | D16   | 450  | GLY  | CA-C-N | 5.02  | 131.14      | 121.54   |
| 24  | D16   | 450  | GLY  | C-N-CA | 5.02  | 131.14      | 121.54   |
| 10  | C32   | 673  | VAL  | CA-C-N | 5.02  | 129.58      | 122.24   |
| 10  | C32   | 673  | VAL  | C-N-CA | 5.02  | 129.58      | 122.24   |
| 1   | R     | 1144 | CYS  | CA-C-N | -5.02 | 114.07      | 123.01   |
| 1   | R     | 1144 | CYS  | C-N-CA | -5.02 | 114.07      | 123.01   |
| 10  | C16   | 1625 | SER  | CA-C-N | 5.02  | 131.13      | 121.54   |
| 10  | C16   | 1625 | SER  | C-N-CA | 5.02  | 131.13      | 121.54   |
| 18  | B     | 795  | ASP  | O-C-N  | -5.02 | 116.90      | 122.93   |
| 18  | B8    | 1311 | TRP  | O-C-N  | -5.02 | 115.91      | 122.39   |
| 18  | B8    | 1747 | SER  | O-C-N  | -5.02 | 113.30      | 122.34   |
| 10  | C24   | 1275 | LEU  | CA-C-N | -5.02 | 113.57      | 122.26   |
| 10  | C24   | 1275 | LEU  | C-N-CA | -5.02 | 113.57      | 122.26   |
| 18  | B8    | 355  | HIS  | CA-C-N | 5.02  | 128.53      | 120.30   |
| 18  | B8    | 355  | HIS  | C-N-CA | 5.02  | 128.53      | 120.30   |
| 20  | E     | 435  | ALA  | CA-C-N | -5.02 | 111.95      | 121.54   |
| 20  | E     | 435  | ALA  | C-N-CA | -5.02 | 111.95      | 121.54   |
| 10  | C32   | 672  | ASP  | CA-C-N | 5.02  | 129.18      | 122.95   |
| 10  | C32   | 672  | ASP  | C-N-CA | 5.02  | 129.18      | 122.95   |
| 2   | M8    | 756  | MET  | O-C-N  | -5.02 | 115.91      | 122.59   |
| 10  | C16   | 429  | SER  | O-C-N  | -5.02 | 116.29      | 122.11   |
| 10  | C     | 1344 | VAL  | O-C-N  | 5.02  | 127.00      | 121.83   |
| 10  | C8    | 1344 | VAL  | O-C-N  | 5.02  | 127.00      | 121.83   |
| 10  | C8    | 1625 | SER  | CA-C-N | 5.02  | 131.13      | 121.54   |
| 10  | C8    | 1625 | SER  | C-N-CA | 5.02  | 131.13      | 121.54   |
| 18  | B8    | 1423 | SER  | CA-C-N | 5.02  | 127.51      | 120.28   |
| 18  | B8    | 1423 | SER  | C-N-CA | 5.02  | 127.51      | 120.28   |
| 24  | D40   | 450  | GLY  | CA-C-N | 5.02  | 131.13      | 121.54   |
| 24  | D40   | 450  | GLY  | C-N-CA | 5.02  | 131.13      | 121.54   |
| 10  | C32   | 898  | GLN  | O-C-N  | 5.02  | 127.44      | 122.12   |
| 1   | R16   | 1484 | VAL  | O-C-N  | 5.02  | 127.00      | 121.83   |
| 9   | K8    | 927  | ARG  | O-C-N  | -5.02 | 115.92      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 10  | C24   | 1498 | GLY  | CA-C-N    | 5.02  | 131.12      | 121.54   |
| 10  | C24   | 1498 | GLY  | C-N-CA    | 5.02  | 131.12      | 121.54   |
| 10  | C16   | 1331 | CYS  | O-C-N     | -5.01 | 115.71      | 122.23   |
| 10  | C16   | 1664 | SER  | O-C-N     | -5.01 | 115.92      | 122.59   |
| 23  | J8    | 729  | ARG  | CA-C-N    | -5.01 | 113.56      | 120.28   |
| 23  | J8    | 729  | ARG  | C-N-CA    | -5.01 | 113.56      | 120.28   |
| 10  | C32   | 1334 | MET  | CA-C-N    | 5.01  | 129.64      | 123.12   |
| 10  | C32   | 1334 | MET  | C-N-CA    | 5.01  | 129.64      | 123.12   |
| 6   | O8    | 51   | LYS  | CA-C-N    | -5.01 | 115.49      | 122.71   |
| 6   | O8    | 51   | LYS  | C-N-CA    | -5.01 | 115.49      | 122.71   |
| 10  | C16   | 1498 | GLY  | CA-C-N    | 5.01  | 131.11      | 121.54   |
| 10  | C16   | 1498 | GLY  | C-N-CA    | 5.01  | 131.11      | 121.54   |
| 2   | M     | 202  | LYS  | O-C-N     | 5.01  | 127.04      | 121.43   |
| 10  | C     | 922  | ALA  | CA-C-N    | -5.01 | 114.57      | 119.93   |
| 10  | C     | 922  | ALA  | C-N-CA    | -5.01 | 114.57      | 119.93   |
| 18  | B8    | 611  | ASN  | CA-C-N    | -5.01 | 115.12      | 120.43   |
| 18  | B8    | 611  | ASN  | C-N-CA    | -5.01 | 115.12      | 120.43   |
| 20  | E     | 2    | PRO  | O-C-N     | -5.01 | 115.88      | 122.64   |
| 24  | D40   | 759  | TYR  | N-CA-C    | 5.01  | 121.47      | 110.80   |
| 24  | D40   | 796  | ARG  | NE-CZ-NH2 | 5.01  | 123.71      | 119.20   |
| 10  | C32   | 306  | ASP  | CA-C-N    | 5.01  | 124.31      | 118.85   |
| 10  | C32   | 306  | ASP  | C-N-CA    | 5.01  | 124.31      | 118.85   |
| 2   | M     | 686  | ILE  | O-C-N     | 5.01  | 126.99      | 121.83   |
| 6   | O     | 51   | LYS  | CA-C-N    | -5.01 | 115.50      | 122.71   |
| 6   | O     | 51   | LYS  | C-N-CA    | -5.01 | 115.50      | 122.71   |
| 10  | C24   | 60   | LYS  | O-C-N     | -5.01 | 116.52      | 121.88   |
| 10  | C24   | 429  | SER  | O-C-N     | -5.01 | 116.30      | 122.11   |
| 10  | C24   | 1344 | VAL  | O-C-N     | 5.01  | 126.99      | 121.83   |
| 18  | B8    | 1392 | SER  | O-C-N     | 5.01  | 128.98      | 122.42   |
| 22  | I24   | 113  | HIS  | CA-C-N    | 5.01  | 125.28      | 119.47   |
| 22  | I24   | 113  | HIS  | C-N-CA    | 5.01  | 125.28      | 119.47   |
| 9   | K     | 1042 | HIS  | O-C-N     | 5.01  | 127.43      | 122.12   |
| 9   | K8    | 792  | LEU  | O-C-N     | 5.01  | 127.86      | 122.15   |
| 9   | K16   | 1284 | MET  | CA-C-N    | 5.01  | 130.72      | 121.70   |
| 9   | K16   | 1284 | MET  | C-N-CA    | 5.01  | 130.72      | 121.70   |
| 13  | V     | 841  | GLN  | O-C-N     | 5.01  | 127.86      | 122.15   |
| 10  | C     | 429  | SER  | O-C-N     | -5.01 | 116.30      | 122.11   |
| 10  | C     | 646  | VAL  | O-C-N     | -5.01 | 116.31      | 122.57   |
| 10  | C8    | 335  | ASP  | O-C-N     | -5.01 | 115.93      | 122.59   |
| 10  | C8    | 1275 | LEU  | CA-C-N    | -5.01 | 113.59      | 122.26   |
| 10  | C8    | 1275 | LEU  | C-N-CA    | -5.01 | 113.59      | 122.26   |
| 2   | M8    | 686  | ILE  | O-C-N     | 5.01  | 126.99      | 121.83   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | T     | 75   | HIS  | N-CA-C     | 5.01  | 117.47      | 111.71   |
| 9   | K     | 897  | LEU  | O-C-N      | 5.01  | 127.86      | 122.15   |
| 10  | C16   | 672  | ASP  | CA-C-N     | 5.01  | 129.16      | 122.95   |
| 10  | C16   | 672  | ASP  | C-N-CA     | 5.01  | 129.16      | 122.95   |
| 10  | C16   | 898  | GLN  | O-C-N      | 5.01  | 127.43      | 122.12   |
| 24  | D8    | 759  | TYR  | N-CA-C     | 5.01  | 121.46      | 110.80   |
| 10  | C32   | 646  | VAL  | O-C-N      | -5.01 | 116.31      | 122.57   |
| 1   | R     | 1386 | MET  | O-C-N      | 5.00  | 128.25      | 122.19   |
| 10  | C8    | 1439 | ILE  | O-C-N      | -5.00 | 117.09      | 122.45   |
| 17  | F8    | 55   | PRO  | O-C-N      | 5.00  | 127.37      | 121.46   |
| 2   | M8    | 460  | TYR  | O-C-N      | 5.00  | 127.85      | 122.15   |
| 2   | M16   | 347  | LYS  | CA-C-N     | -5.00 | 111.98      | 121.54   |
| 2   | M16   | 347  | LYS  | C-N-CA     | -5.00 | 111.98      | 121.54   |
| 4   | T     | 126  | GLN  | OE1-CD-NE2 | -5.00 | 117.60      | 122.60   |
| 10  | C16   | 1439 | ILE  | O-C-N      | -5.00 | 117.10      | 122.45   |
| 10  | C     | 1625 | SER  | CA-C-N     | 5.00  | 131.10      | 121.54   |
| 10  | C     | 1625 | SER  | C-N-CA     | 5.00  | 131.10      | 121.54   |
| 18  | B     | 1311 | TRP  | O-C-N      | -5.00 | 115.94      | 122.39   |
| 22  | I24   | 204  | PRO  | O-C-N      | -5.00 | 115.52      | 122.37   |
| 22  | I16   | 297  | HIS  | O-C-N      | -5.00 | 115.93      | 122.59   |
| 24  | D32   | 1069 | GLY  | CA-C-N     | 5.00  | 127.88      | 120.82   |
| 24  | D32   | 1069 | GLY  | C-N-CA     | 5.00  | 127.88      | 120.82   |
| 2   | M     | 347  | LYS  | CA-C-N     | -5.00 | 111.99      | 121.54   |
| 2   | M     | 347  | LYS  | C-N-CA     | -5.00 | 111.99      | 121.54   |
| 10  | C24   | 1164 | VAL  | O-C-N      | -5.00 | 116.99      | 121.89   |
| 10  | C8    | 581  | TYR  | O-C-N      | -5.00 | 117.52      | 123.22   |
| 22  | I24   | 345  | GLU  | O-C-N      | -5.00 | 116.93      | 122.93   |

There are no chirality outliers.

All (2705) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 19  | 4     | 100 | ILE  | Mainchain |
| 19  | 4     | 102 | LEU  | Mainchain |
| 19  | 4     | 103 | GLN  | Mainchain |
| 19  | 4     | 185 | GLY  | Mainchain |
| 19  | 4     | 186 | GLY  | Mainchain |
| 19  | 4     | 187 | SER  | Mainchain |
| 19  | 4     | 188 | ALA  | Mainchain |
| 19  | 4     | 189 | LEU  | Mainchain |
| 19  | 4     | 192 | SER  | Mainchain |
| 19  | 4     | 193 | LEU  | Mainchain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 19  | 4     | 194 | SER  | Mainchain         |
| 19  | 4     | 195 | ARG  | Mainchain         |
| 19  | 4     | 196 | GLY  | Mainchain         |
| 19  | 4     | 445 | VAL  | Mainchain         |
| 19  | 4     | 47  | PHE  | Mainchain         |
| 19  | 4     | 48  | ASP  | Mainchain         |
| 19  | 4     | 50  | THR  | Mainchain         |
| 19  | 4     | 51  | PRO  | Mainchain         |
| 19  | 4     | 52  | SER  | Mainchain         |
| 19  | 4     | 53  | SER  | Mainchain         |
| 19  | 4     | 54  | LEU  | Mainchain         |
| 19  | 4     | 55  | GLN  | Mainchain         |
| 19  | 4     | 56  | GLU  | Mainchain         |
| 19  | 4     | 57  | ASN  | Mainchain         |
| 19  | 4     | 58  | GLU  | Mainchain         |
| 19  | 4     | 59  | GLY  | Mainchain         |
| 19  | 4     | 60  | GLN  | Mainchain         |
| 19  | 4     | 61  | GLU  | Mainchain         |
| 19  | 4     | 62  | ASN  | Mainchain         |
| 19  | 4     | 63  | GLY  | Mainchain         |
| 19  | 4     | 64  | ASP  | Mainchain         |
| 19  | 4     | 66  | ALA  | Peptide,Mainchain |
| 19  | 4     | 67  | SER  | Peptide,Mainchain |
| 19  | 4     | 68  | GLY  | Mainchain         |
| 19  | 4     | 69  | GLU  | Peptide,Mainchain |
| 19  | 4     | 70  | SER  | Mainchain         |
| 19  | 4     | 90  | GLN  | Mainchain         |
| 19  | 4     | 91  | PRO  | Mainchain         |
| 19  | 4     | 92  | THR  | Mainchain         |
| 19  | 4     | 93  | ASP  | Mainchain         |
| 19  | 48    | 100 | ILE  | Mainchain         |
| 19  | 48    | 102 | LEU  | Mainchain         |
| 19  | 48    | 103 | GLN  | Mainchain         |
| 19  | 48    | 185 | GLY  | Mainchain         |
| 19  | 48    | 186 | GLY  | Mainchain         |
| 19  | 48    | 187 | SER  | Mainchain         |
| 19  | 48    | 188 | ALA  | Mainchain         |
| 19  | 48    | 189 | LEU  | Mainchain         |
| 19  | 48    | 192 | SER  | Mainchain         |
| 19  | 48    | 193 | LEU  | Mainchain         |
| 19  | 48    | 194 | SER  | Mainchain         |
| 19  | 48    | 195 | ARG  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 19  | 48    | 196 | GLY  | Mainchain         |
| 19  | 48    | 445 | VAL  | Mainchain         |
| 19  | 48    | 47  | PHE  | Mainchain         |
| 19  | 48    | 48  | ASP  | Mainchain         |
| 19  | 48    | 50  | THR  | Mainchain         |
| 19  | 48    | 51  | PRO  | Mainchain         |
| 19  | 48    | 52  | SER  | Mainchain         |
| 19  | 48    | 53  | SER  | Mainchain         |
| 19  | 48    | 54  | LEU  | Mainchain         |
| 19  | 48    | 55  | GLN  | Mainchain         |
| 19  | 48    | 56  | GLU  | Mainchain         |
| 19  | 48    | 57  | ASN  | Mainchain         |
| 19  | 48    | 58  | GLU  | Mainchain         |
| 19  | 48    | 59  | GLY  | Mainchain         |
| 19  | 48    | 60  | GLN  | Mainchain         |
| 19  | 48    | 61  | GLU  | Mainchain         |
| 19  | 48    | 62  | ASN  | Mainchain         |
| 19  | 48    | 63  | GLY  | Mainchain         |
| 19  | 48    | 64  | ASP  | Mainchain         |
| 19  | 48    | 66  | ALA  | Peptide,Mainchain |
| 19  | 48    | 67  | SER  | Peptide,Mainchain |
| 19  | 48    | 68  | GLY  | Mainchain         |
| 19  | 48    | 69  | GLU  | Peptide,Mainchain |
| 19  | 48    | 70  | SER  | Mainchain         |
| 19  | 48    | 90  | GLN  | Mainchain         |
| 19  | 48    | 91  | PRO  | Mainchain         |
| 19  | 48    | 92  | THR  | Mainchain         |
| 19  | 48    | 93  | ASP  | Mainchain         |
| 12  | A     | 157 | LEU  | Mainchain         |
| 12  | A     | 158 | PRO  | Mainchain         |
| 12  | A     | 159 | LYS  | Mainchain         |
| 12  | A     | 237 | LEU  | Mainchain         |
| 12  | A     | 239 | ALA  | Mainchain         |
| 12  | A     | 240 | GLU  | Mainchain         |
| 12  | A     | 241 | VAL  | Mainchain         |
| 12  | A     | 242 | THR  | Mainchain         |
| 12  | A     | 243 | ARG  | Mainchain         |
| 12  | A     | 265 | ALA  | Mainchain         |
| 12  | A     | 268 | GLN  | Mainchain         |
| 12  | A     | 309 | VAL  | Mainchain         |
| 12  | A     | 461 | VAL  | Mainchain         |
| 12  | A     | 462 | THR  | Mainchain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 12  | A     | 463 | GLY  | Mainchain |
| 12  | A     | 464 | GLY  | Mainchain |
| 12  | A     | 465 | SER  | Mainchain |
| 12  | A     | 466 | SER  | Mainchain |
| 12  | A     | 467 | SER  | Mainchain |
| 12  | A     | 468 | VAL  | Mainchain |
| 12  | A     | 469 | VAL  | Mainchain |
| 12  | A     | 470 | LEU  | Mainchain |
| 12  | A     | 471 | ASN  | Mainchain |
| 12  | A     | 473 | GLY  | Mainchain |
| 12  | A     | 525 | ALA  | Mainchain |
| 12  | A     | 551 | SER  | Mainchain |
| 12  | A     | 552 | GLY  | Mainchain |
| 12  | A     | 555 | HIS  | Mainchain |
| 12  | A     | 556 | LYS  | Mainchain |
| 12  | A     | 558 | SER  | Mainchain |
| 12  | A     | 560 | MET  | Mainchain |
| 12  | A     | 782 | PRO  | Mainchain |
| 12  | A     | 794 | THR  | Mainchain |
| 12  | A     | 795 | ALA  | Mainchain |
| 12  | A     | 796 | ASP  | Mainchain |
| 12  | A     | 847 | ARG  | Mainchain |
| 11  | A16   | 1   | MET  | Mainchain |
| 11  | A16   | 159 | LYS  | Mainchain |
| 11  | A16   | 237 | LEU  | Mainchain |
| 11  | A16   | 239 | ALA  | Mainchain |
| 11  | A16   | 240 | GLU  | Mainchain |
| 11  | A16   | 241 | VAL  | Mainchain |
| 11  | A16   | 242 | THR  | Mainchain |
| 11  | A16   | 243 | ARG  | Mainchain |
| 11  | A16   | 265 | ALA  | Mainchain |
| 11  | A16   | 268 | GLN  | Mainchain |
| 11  | A16   | 28  | SER  | Mainchain |
| 11  | A16   | 309 | VAL  | Mainchain |
| 11  | A16   | 461 | VAL  | Mainchain |
| 11  | A16   | 462 | THR  | Mainchain |
| 11  | A16   | 463 | GLY  | Mainchain |
| 11  | A16   | 464 | GLY  | Mainchain |
| 11  | A16   | 465 | SER  | Mainchain |
| 11  | A16   | 466 | SER  | Mainchain |
| 11  | A16   | 467 | SER  | Mainchain |
| 11  | A16   | 468 | VAL  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 11  | A16   | 469 | VAL  | Mainchain |
| 11  | A16   | 470 | LEU  | Mainchain |
| 11  | A16   | 471 | ASN  | Mainchain |
| 11  | A16   | 473 | GLY  | Mainchain |
| 11  | A16   | 525 | ALA  | Mainchain |
| 11  | A16   | 54  | ASN  | Mainchain |
| 11  | A16   | 551 | SER  | Mainchain |
| 11  | A16   | 552 | GLY  | Mainchain |
| 11  | A16   | 555 | HIS  | Mainchain |
| 11  | A16   | 556 | LYS  | Mainchain |
| 11  | A16   | 558 | SER  | Mainchain |
| 11  | A16   | 56  | ALA  | Mainchain |
| 11  | A16   | 560 | MET  | Mainchain |
| 11  | A16   | 782 | PRO  | Mainchain |
| 11  | A16   | 794 | THR  | Mainchain |
| 11  | A16   | 795 | ALA  | Mainchain |
| 11  | A16   | 796 | ASP  | Mainchain |
| 11  | A16   | 847 | ARG  | Mainchain |
| 11  | A24   | 1   | MET  | Mainchain |
| 11  | A24   | 157 | LEU  | Mainchain |
| 11  | A24   | 158 | PRO  | Mainchain |
| 11  | A24   | 159 | LYS  | Mainchain |
| 11  | A24   | 237 | LEU  | Mainchain |
| 11  | A24   | 239 | ALA  | Mainchain |
| 11  | A24   | 240 | GLU  | Mainchain |
| 11  | A24   | 241 | VAL  | Mainchain |
| 11  | A24   | 242 | THR  | Mainchain |
| 11  | A24   | 243 | ARG  | Mainchain |
| 11  | A24   | 265 | ALA  | Mainchain |
| 11  | A24   | 268 | GLN  | Mainchain |
| 11  | A24   | 28  | SER  | Mainchain |
| 11  | A24   | 309 | VAL  | Mainchain |
| 11  | A24   | 461 | VAL  | Mainchain |
| 11  | A24   | 462 | THR  | Mainchain |
| 11  | A24   | 463 | GLY  | Mainchain |
| 11  | A24   | 464 | GLY  | Mainchain |
| 11  | A24   | 465 | SER  | Mainchain |
| 11  | A24   | 466 | SER  | Mainchain |
| 11  | A24   | 467 | SER  | Mainchain |
| 11  | A24   | 468 | VAL  | Mainchain |
| 11  | A24   | 469 | VAL  | Mainchain |
| 11  | A24   | 470 | LEU  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 11  | A24   | 471 | ASN  | Mainchain |
| 11  | A24   | 473 | GLY  | Mainchain |
| 11  | A24   | 525 | ALA  | Mainchain |
| 11  | A24   | 54  | ASN  | Mainchain |
| 11  | A24   | 551 | SER  | Mainchain |
| 11  | A24   | 552 | GLY  | Mainchain |
| 11  | A24   | 555 | HIS  | Mainchain |
| 11  | A24   | 556 | LYS  | Mainchain |
| 11  | A24   | 558 | SER  | Mainchain |
| 11  | A24   | 56  | ALA  | Mainchain |
| 11  | A24   | 560 | MET  | Mainchain |
| 11  | A24   | 782 | PRO  | Mainchain |
| 11  | A24   | 794 | THR  | Mainchain |
| 11  | A24   | 795 | ALA  | Mainchain |
| 11  | A24   | 796 | ASP  | Mainchain |
| 11  | A24   | 847 | ARG  | Mainchain |
| 11  | A32   | 1   | MET  | Mainchain |
| 11  | A32   | 159 | LYS  | Mainchain |
| 11  | A32   | 237 | LEU  | Mainchain |
| 11  | A32   | 239 | ALA  | Mainchain |
| 11  | A32   | 240 | GLU  | Mainchain |
| 11  | A32   | 241 | VAL  | Mainchain |
| 11  | A32   | 242 | THR  | Mainchain |
| 11  | A32   | 243 | ARG  | Mainchain |
| 11  | A32   | 265 | ALA  | Mainchain |
| 11  | A32   | 268 | GLN  | Mainchain |
| 11  | A32   | 28  | SER  | Mainchain |
| 11  | A32   | 309 | VAL  | Mainchain |
| 11  | A32   | 461 | VAL  | Mainchain |
| 11  | A32   | 462 | THR  | Mainchain |
| 11  | A32   | 463 | GLY  | Mainchain |
| 11  | A32   | 464 | GLY  | Mainchain |
| 11  | A32   | 465 | SER  | Mainchain |
| 11  | A32   | 466 | SER  | Mainchain |
| 11  | A32   | 467 | SER  | Mainchain |
| 11  | A32   | 468 | VAL  | Mainchain |
| 11  | A32   | 469 | VAL  | Mainchain |
| 11  | A32   | 470 | LEU  | Mainchain |
| 11  | A32   | 471 | ASN  | Mainchain |
| 11  | A32   | 473 | GLY  | Mainchain |
| 11  | A32   | 525 | ALA  | Mainchain |
| 11  | A32   | 54  | ASN  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 11  | A32   | 551 | SER  | Mainchain |
| 11  | A32   | 552 | GLY  | Mainchain |
| 11  | A32   | 555 | HIS  | Mainchain |
| 11  | A32   | 556 | LYS  | Mainchain |
| 11  | A32   | 558 | SER  | Mainchain |
| 11  | A32   | 56  | ALA  | Mainchain |
| 11  | A32   | 560 | MET  | Mainchain |
| 11  | A32   | 782 | PRO  | Mainchain |
| 11  | A32   | 794 | THR  | Mainchain |
| 11  | A32   | 795 | ALA  | Mainchain |
| 11  | A32   | 796 | ASP  | Mainchain |
| 11  | A32   | 847 | ARG  | Mainchain |
| 11  | A40   | 1   | MET  | Mainchain |
| 11  | A40   | 157 | LEU  | Mainchain |
| 11  | A40   | 158 | PRO  | Mainchain |
| 11  | A40   | 159 | LYS  | Mainchain |
| 11  | A40   | 237 | LEU  | Mainchain |
| 11  | A40   | 239 | ALA  | Mainchain |
| 11  | A40   | 240 | GLU  | Mainchain |
| 11  | A40   | 241 | VAL  | Mainchain |
| 11  | A40   | 242 | THR  | Mainchain |
| 11  | A40   | 243 | ARG  | Mainchain |
| 11  | A40   | 265 | ALA  | Mainchain |
| 11  | A40   | 268 | GLN  | Mainchain |
| 11  | A40   | 28  | SER  | Mainchain |
| 11  | A40   | 309 | VAL  | Mainchain |
| 11  | A40   | 461 | VAL  | Mainchain |
| 11  | A40   | 462 | THR  | Mainchain |
| 11  | A40   | 463 | GLY  | Mainchain |
| 11  | A40   | 464 | GLY  | Mainchain |
| 11  | A40   | 465 | SER  | Mainchain |
| 11  | A40   | 466 | SER  | Mainchain |
| 11  | A40   | 467 | SER  | Mainchain |
| 11  | A40   | 468 | VAL  | Mainchain |
| 11  | A40   | 469 | VAL  | Mainchain |
| 11  | A40   | 470 | LEU  | Mainchain |
| 11  | A40   | 471 | ASN  | Mainchain |
| 11  | A40   | 473 | GLY  | Mainchain |
| 11  | A40   | 525 | ALA  | Mainchain |
| 11  | A40   | 54  | ASN  | Mainchain |
| 11  | A40   | 551 | SER  | Mainchain |
| 11  | A40   | 552 | GLY  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 11  | A40   | 555 | HIS  | Mainchain |
| 11  | A40   | 556 | LYS  | Mainchain |
| 11  | A40   | 558 | SER  | Mainchain |
| 11  | A40   | 56  | ALA  | Mainchain |
| 11  | A40   | 560 | MET  | Mainchain |
| 11  | A40   | 782 | PRO  | Mainchain |
| 11  | A40   | 794 | THR  | Mainchain |
| 11  | A40   | 795 | ALA  | Mainchain |
| 11  | A40   | 796 | ASP  | Mainchain |
| 11  | A40   | 847 | ARG  | Mainchain |
| 12  | A48   | 157 | LEU  | Mainchain |
| 12  | A48   | 158 | PRO  | Mainchain |
| 12  | A48   | 159 | LYS  | Mainchain |
| 12  | A48   | 237 | LEU  | Mainchain |
| 12  | A48   | 239 | ALA  | Mainchain |
| 12  | A48   | 240 | GLU  | Mainchain |
| 12  | A48   | 241 | VAL  | Mainchain |
| 12  | A48   | 242 | THR  | Mainchain |
| 12  | A48   | 243 | ARG  | Mainchain |
| 12  | A48   | 265 | ALA  | Mainchain |
| 12  | A48   | 268 | GLN  | Mainchain |
| 12  | A48   | 309 | VAL  | Mainchain |
| 12  | A48   | 461 | VAL  | Mainchain |
| 12  | A48   | 462 | THR  | Mainchain |
| 12  | A48   | 463 | GLY  | Mainchain |
| 12  | A48   | 464 | GLY  | Mainchain |
| 12  | A48   | 465 | SER  | Mainchain |
| 12  | A48   | 466 | SER  | Mainchain |
| 12  | A48   | 467 | SER  | Mainchain |
| 12  | A48   | 468 | VAL  | Mainchain |
| 12  | A48   | 469 | VAL  | Mainchain |
| 12  | A48   | 470 | LEU  | Mainchain |
| 12  | A48   | 471 | ASN  | Mainchain |
| 12  | A48   | 473 | GLY  | Mainchain |
| 12  | A48   | 525 | ALA  | Mainchain |
| 12  | A48   | 551 | SER  | Mainchain |
| 12  | A48   | 552 | GLY  | Mainchain |
| 12  | A48   | 555 | HIS  | Mainchain |
| 12  | A48   | 556 | LYS  | Mainchain |
| 12  | A48   | 558 | SER  | Mainchain |
| 12  | A48   | 560 | MET  | Mainchain |
| 12  | A48   | 782 | PRO  | Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 12  | A48   | 794  | THR  | Mainchain         |
| 12  | A48   | 795  | ALA  | Mainchain         |
| 12  | A48   | 796  | ASP  | Mainchain         |
| 12  | A48   | 847  | ARG  | Mainchain         |
| 16  | A8    | 157  | LEU  | Mainchain         |
| 16  | A8    | 158  | PRO  | Mainchain         |
| 16  | A8    | 159  | LYS  | Mainchain         |
| 18  | B     | 1    | MET  | Mainchain         |
| 18  | B     | 1064 | ILE  | Mainchain         |
| 18  | B     | 1066 | ASP  | Mainchain         |
| 18  | B     | 1067 | SER  | Mainchain         |
| 18  | B     | 1068 | THR  | Mainchain         |
| 18  | B     | 1111 | LYS  | Mainchain         |
| 18  | B     | 1113 | PRO  | Mainchain         |
| 18  | B     | 1114 | CYS  | Mainchain         |
| 18  | B     | 1116 | GLU  | Mainchain         |
| 18  | B     | 1119 | LYS  | Peptide,Mainchain |
| 18  | B     | 1122 | SER  | Mainchain         |
| 18  | B     | 1124 | GLY  | Mainchain         |
| 18  | B     | 1125 | VAL  | Mainchain         |
| 18  | B     | 1126 | SER  | Mainchain         |
| 18  | B     | 1127 | PRO  | Mainchain         |
| 18  | B     | 1128 | PRO  | Mainchain         |
| 18  | B     | 1129 | LYS  | Mainchain         |
| 18  | B     | 113  | TYR  | Mainchain         |
| 18  | B     | 1130 | LEU  | Mainchain         |
| 18  | B     | 1131 | THR  | Mainchain         |
| 18  | B     | 1132 | TRP  | Mainchain         |
| 18  | B     | 1133 | THR  | Mainchain         |
| 18  | B     | 116  | THR  | Mainchain         |
| 18  | B     | 1161 | LEU  | Mainchain         |
| 18  | B     | 118  | SER  | Mainchain         |
| 18  | B     | 121  | GLN  | Mainchain         |
| 18  | B     | 122  | GLU  | Mainchain         |
| 18  | B     | 1225 | LEU  | Mainchain         |
| 18  | B     | 1227 | TYR  | Mainchain         |
| 18  | B     | 1228 | SER  | Mainchain         |
| 18  | B     | 1229 | GLY  | Mainchain         |
| 18  | B     | 123  | LEU  | Mainchain         |
| 18  | B     | 1231 | LYS  | Mainchain         |
| 18  | B     | 124  | THR  | Mainchain         |
| 18  | B     | 1276 | LYS  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B     | 1277 | GLN  | Mainchain         |
| 18  | B     | 1278 | LYS  | Mainchain         |
| 18  | B     | 1279 | THR  | Mainchain         |
| 18  | B     | 1280 | ASN  | Mainchain         |
| 18  | B     | 1283 | VAL  | Mainchain         |
| 18  | B     | 1284 | ASN  | Mainchain         |
| 18  | B     | 1287 | LEU  | Mainchain         |
| 18  | B     | 1288 | GLY  | Mainchain         |
| 18  | B     | 1289 | ASP  | Mainchain         |
| 18  | B     | 1358 | GLU  | Mainchain         |
| 18  | B     | 1360 | SER  | Mainchain         |
| 18  | B     | 1362 | ALA  | Mainchain         |
| 18  | B     | 1363 | ALA  | Mainchain         |
| 18  | B     | 1364 | GLU  | Mainchain         |
| 18  | B     | 1365 | ARG  | Mainchain         |
| 18  | B     | 1420 | LYS  | Mainchain         |
| 18  | B     | 1444 | LEU  | Mainchain         |
| 18  | B     | 1446 | HIS  | Mainchain         |
| 18  | B     | 1447 | SER  | Mainchain         |
| 18  | B     | 1476 | SER  | Mainchain         |
| 18  | B     | 1477 | GLY  | Mainchain         |
| 18  | B     | 1478 | MET  | Peptide,Mainchain |
| 18  | B     | 1479 | GLY  | Mainchain         |
| 18  | B     | 1483 | LEU  | Mainchain         |
| 18  | B     | 1552 | LYS  | Mainchain         |
| 18  | B     | 1593 | PHE  | Mainchain         |
| 18  | B     | 1594 | PRO  | Mainchain         |
| 18  | B     | 1595 | ASP  | Mainchain         |
| 18  | B     | 1596 | GLY  | Mainchain         |
| 18  | B     | 1597 | MET  | Mainchain         |
| 18  | B     | 1601 | VAL  | Mainchain         |
| 18  | B     | 1602 | SER  | Mainchain         |
| 18  | B     | 1603 | ASP  | Peptide,Mainchain |
| 18  | B     | 1604 | ASN  | Mainchain         |
| 18  | B     | 1605 | GLU  | Peptide,Mainchain |
| 18  | B     | 1606 | LYS  | Peptide,Mainchain |
| 18  | B     | 1637 | VAL  | Mainchain         |
| 18  | B     | 1669 | PRO  | Mainchain         |
| 18  | B     | 1670 | SER  | Mainchain         |
| 18  | B     | 1671 | ASP  | Mainchain         |
| 18  | B     | 1672 | ASP  | Mainchain         |
| 18  | B     | 1673 | ARG  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B     | 1674 | ASP  | Mainchain         |
| 18  | B     | 1675 | LYS  | Mainchain         |
| 18  | B     | 1676 | VAL  | Mainchain         |
| 18  | B     | 1677 | ARG  | Mainchain         |
| 18  | B     | 1678 | LEU  | Mainchain         |
| 18  | B     | 1679 | ARG  | Mainchain         |
| 18  | B     | 1680 | SER  | Mainchain         |
| 18  | B     | 1681 | GLN  | Mainchain         |
| 18  | B     | 1682 | ARG  | Mainchain         |
| 18  | B     | 1683 | THR  | Mainchain         |
| 18  | B     | 1685 | THR  | Mainchain         |
| 18  | B     | 1742 | SER  | Mainchain         |
| 18  | B     | 1747 | SER  | Mainchain         |
| 18  | B     | 1783 | VAL  | Mainchain         |
| 18  | B     | 1784 | GLY  | Mainchain         |
| 18  | B     | 1785 | LYS  | Mainchain         |
| 18  | B     | 1786 | PRO  | Mainchain         |
| 18  | B     | 1787 | LYS  | Mainchain         |
| 18  | B     | 1788 | ILE  | Mainchain         |
| 18  | B     | 1789 | THR  | Mainchain         |
| 18  | B     | 1790 | ALA  | Mainchain         |
| 18  | B     | 1791 | VAL  | Mainchain         |
| 18  | B     | 1792 | SER  | Mainchain         |
| 18  | B     | 1793 | ILE  | Mainchain         |
| 18  | B     | 1794 | SER  | Mainchain         |
| 18  | B     | 1797 | LEU  | Peptide,Mainchain |
| 18  | B     | 1798 | VAL  | Peptide           |
| 18  | B     | 1799 | VAL  | Mainchain         |
| 18  | B     | 1800 | ARG  | Mainchain         |
| 18  | B     | 1801 | GLY  | Mainchain         |
| 18  | B     | 1802 | ASP  | Mainchain         |
| 18  | B     | 1803 | THR  | Mainchain         |
| 18  | B     | 1804 | THR  | Mainchain         |
| 18  | B     | 1806 | HIS  | Mainchain         |
| 18  | B     | 1807 | PRO  | Mainchain         |
| 18  | B     | 1808 | GLY  | Mainchain         |
| 18  | B     | 1809 | SER  | Mainchain         |
| 18  | B     | 192  | PRO  | Mainchain         |
| 18  | B     | 2    | ALA  | Mainchain         |
| 18  | B     | 249  | TYR  | Mainchain         |
| 18  | B     | 298  | THR  | Mainchain         |
| 18  | B     | 384  | ASP  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 18  | B     | 4   | PRO  | Mainchain         |
| 18  | B     | 413 | ASP  | Mainchain         |
| 18  | B     | 499 | ILE  | Mainchain         |
| 18  | B     | 500 | THR  | Mainchain         |
| 18  | B     | 504 | PRO  | Mainchain         |
| 18  | B     | 505 | ALA  | Mainchain         |
| 18  | B     | 506 | ASP  | Mainchain         |
| 18  | B     | 508 | ALA  | Mainchain         |
| 18  | B     | 606 | GLN  | Mainchain         |
| 18  | B     | 608 | SER  | Mainchain         |
| 18  | B     | 609 | TYR  | Mainchain         |
| 18  | B     | 610 | VAL  | Mainchain         |
| 18  | B     | 611 | ASN  | Mainchain         |
| 18  | B     | 612 | GLY  | Mainchain         |
| 18  | B     | 613 | LYS  | Mainchain         |
| 18  | B     | 614 | MET  | Mainchain         |
| 18  | B     | 617 | ASP  | Mainchain         |
| 18  | B     | 671 | MET  | Mainchain         |
| 18  | B     | 672 | THR  | Mainchain         |
| 18  | B     | 673 | SER  | Mainchain         |
| 18  | B     | 674 | CYS  | Mainchain         |
| 18  | B     | 675 | SER  | Mainchain         |
| 18  | B     | 676 | ASP  | Mainchain         |
| 18  | B     | 677 | VAL  | Mainchain         |
| 18  | B     | 679 | ASP  | Mainchain         |
| 18  | B     | 681 | GLY  | Peptide,Mainchain |
| 18  | B     | 682 | TYR  | Mainchain         |
| 18  | B     | 683 | ASN  | Mainchain         |
| 18  | B     | 684 | ILE  | Mainchain         |
| 18  | B     | 685 | SER  | Mainchain         |
| 18  | B     | 688 | GLY  | Mainchain         |
| 18  | B     | 689 | SER  | Mainchain         |
| 18  | B     | 690 | TRP  | Mainchain         |
| 18  | B     | 691 | SER  | Mainchain         |
| 18  | B     | 693 | SER  | Mainchain         |
| 18  | B     | 854 | SER  | Mainchain         |
| 18  | B     | 855 | GLY  | Mainchain         |
| 18  | B     | 907 | SER  | Mainchain         |
| 18  | B     | 913 | SER  | Mainchain         |
| 18  | B     | 914 | ASN  | Mainchain         |
| 18  | B     | 915 | ALA  | Mainchain         |
| 18  | B     | 969 | ASP  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B     | 970  | SER  | Mainchain         |
| 18  | B     | 974  | SER  | Mainchain         |
| 18  | B     | 975  | ASP  | Mainchain         |
| 18  | B     | 976  | SER  | Mainchain         |
| 18  | B     | 977  | SER  | Peptide,Mainchain |
| 18  | B     | 978  | ASN  | Peptide,Mainchain |
| 18  | B     | 979  | VAL  | Mainchain         |
| 18  | B     | 980  | LYS  | Peptide,Mainchain |
| 18  | B     | 981  | GLN  | Peptide,Mainchain |
| 18  | B     | 982  | SER  | Peptide,Mainchain |
| 18  | B     | 983  | ARG  | Mainchain         |
| 18  | B     | 984  | LYS  | Peptide,Mainchain |
| 18  | B     | 985  | ASP  | Peptide,Mainchain |
| 18  | B     | 987  | SER  | Mainchain         |
| 18  | B     | 988  | SER  | Mainchain         |
| 18  | B     | 989  | ILE  | Mainchain         |
| 18  | B     | 990  | PRO  | Mainchain         |
| 18  | B     | 991  | ASP  | Mainchain         |
| 18  | B     | 992  | TRP  | Mainchain         |
| 18  | B     | 993  | ALA  | Mainchain         |
| 18  | B     | 994  | CYS  | Mainchain         |
| 18  | B8    | 1    | MET  | Mainchain         |
| 18  | B8    | 1064 | ILE  | Mainchain         |
| 18  | B8    | 1065 | LYS  | Mainchain         |
| 18  | B8    | 1066 | ASP  | Mainchain         |
| 18  | B8    | 1067 | SER  | Mainchain         |
| 18  | B8    | 1068 | THR  | Mainchain         |
| 18  | B8    | 1111 | LYS  | Mainchain         |
| 18  | B8    | 1113 | PRO  | Mainchain         |
| 18  | B8    | 1114 | CYS  | Mainchain         |
| 18  | B8    | 1116 | GLU  | Mainchain         |
| 18  | B8    | 1119 | LYS  | Peptide,Mainchain |
| 18  | B8    | 1122 | SER  | Mainchain         |
| 18  | B8    | 1124 | GLY  | Mainchain         |
| 18  | B8    | 1125 | VAL  | Mainchain         |
| 18  | B8    | 1126 | SER  | Mainchain         |
| 18  | B8    | 1127 | PRO  | Mainchain         |
| 18  | B8    | 1128 | PRO  | Mainchain         |
| 18  | B8    | 1129 | LYS  | Mainchain         |
| 18  | B8    | 113  | TYR  | Mainchain         |
| 18  | B8    | 1130 | LEU  | Mainchain         |
| 18  | B8    | 1131 | THR  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B8    | 1132 | TRP  | Mainchain         |
| 18  | B8    | 1133 | THR  | Mainchain         |
| 18  | B8    | 116  | THR  | Mainchain         |
| 18  | B8    | 1161 | LEU  | Mainchain         |
| 18  | B8    | 118  | SER  | Mainchain         |
| 18  | B8    | 121  | GLN  | Mainchain         |
| 18  | B8    | 122  | GLU  | Mainchain         |
| 18  | B8    | 1225 | LEU  | Mainchain         |
| 18  | B8    | 1227 | TYR  | Mainchain         |
| 18  | B8    | 1228 | SER  | Mainchain         |
| 18  | B8    | 1229 | GLY  | Mainchain         |
| 18  | B8    | 123  | LEU  | Mainchain         |
| 18  | B8    | 1231 | LYS  | Mainchain         |
| 18  | B8    | 124  | THR  | Mainchain         |
| 18  | B8    | 1276 | LYS  | Mainchain         |
| 18  | B8    | 1277 | GLN  | Mainchain         |
| 18  | B8    | 1278 | LYS  | Mainchain         |
| 18  | B8    | 1279 | THR  | Mainchain         |
| 18  | B8    | 1280 | ASN  | Mainchain         |
| 18  | B8    | 1283 | VAL  | Mainchain         |
| 18  | B8    | 1284 | ASN  | Mainchain         |
| 18  | B8    | 1287 | LEU  | Mainchain         |
| 18  | B8    | 1288 | GLY  | Mainchain         |
| 18  | B8    | 1289 | ASP  | Mainchain         |
| 18  | B8    | 1358 | GLU  | Mainchain         |
| 18  | B8    | 1360 | SER  | Mainchain         |
| 18  | B8    | 1362 | ALA  | Mainchain         |
| 18  | B8    | 1363 | ALA  | Mainchain         |
| 18  | B8    | 1364 | GLU  | Mainchain         |
| 18  | B8    | 1365 | ARG  | Mainchain         |
| 18  | B8    | 1420 | LYS  | Mainchain         |
| 18  | B8    | 1444 | LEU  | Mainchain         |
| 18  | B8    | 1446 | HIS  | Mainchain         |
| 18  | B8    | 1447 | SER  | Mainchain         |
| 18  | B8    | 1476 | SER  | Mainchain         |
| 18  | B8    | 1477 | GLY  | Mainchain         |
| 18  | B8    | 1478 | MET  | Peptide,Mainchain |
| 18  | B8    | 1479 | GLY  | Mainchain         |
| 18  | B8    | 1481 | MET  | Mainchain         |
| 18  | B8    | 1483 | LEU  | Mainchain         |
| 18  | B8    | 1552 | LYS  | Mainchain         |
| 18  | B8    | 1593 | PHE  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B8    | 1594 | PRO  | Mainchain         |
| 18  | B8    | 1595 | ASP  | Mainchain         |
| 18  | B8    | 1596 | GLY  | Mainchain         |
| 18  | B8    | 1597 | MET  | Mainchain         |
| 18  | B8    | 1601 | VAL  | Mainchain         |
| 18  | B8    | 1602 | SER  | Mainchain         |
| 18  | B8    | 1603 | ASP  | Peptide,Mainchain |
| 18  | B8    | 1604 | ASN  | Mainchain         |
| 18  | B8    | 1605 | GLU  | Peptide,Mainchain |
| 18  | B8    | 1606 | LYS  | Peptide,Mainchain |
| 18  | B8    | 1637 | VAL  | Mainchain         |
| 18  | B8    | 1669 | PRO  | Mainchain         |
| 18  | B8    | 1670 | SER  | Mainchain         |
| 18  | B8    | 1671 | ASP  | Mainchain         |
| 18  | B8    | 1672 | ASP  | Mainchain         |
| 18  | B8    | 1673 | ARG  | Mainchain         |
| 18  | B8    | 1674 | ASP  | Mainchain         |
| 18  | B8    | 1675 | LYS  | Mainchain         |
| 18  | B8    | 1676 | VAL  | Mainchain         |
| 18  | B8    | 1677 | ARG  | Mainchain         |
| 18  | B8    | 1678 | LEU  | Mainchain         |
| 18  | B8    | 1679 | ARG  | Mainchain         |
| 18  | B8    | 1680 | SER  | Mainchain         |
| 18  | B8    | 1681 | GLN  | Mainchain         |
| 18  | B8    | 1682 | ARG  | Mainchain         |
| 18  | B8    | 1683 | THR  | Mainchain         |
| 18  | B8    | 1685 | THR  | Mainchain         |
| 18  | B8    | 1742 | SER  | Mainchain         |
| 18  | B8    | 1747 | SER  | Mainchain         |
| 18  | B8    | 1783 | VAL  | Mainchain         |
| 18  | B8    | 1784 | GLY  | Mainchain         |
| 18  | B8    | 1785 | LYS  | Mainchain         |
| 18  | B8    | 1786 | PRO  | Mainchain         |
| 18  | B8    | 1787 | LYS  | Mainchain         |
| 18  | B8    | 1788 | ILE  | Mainchain         |
| 18  | B8    | 1789 | THR  | Mainchain         |
| 18  | B8    | 1790 | ALA  | Mainchain         |
| 18  | B8    | 1791 | VAL  | Mainchain         |
| 18  | B8    | 1792 | SER  | Mainchain         |
| 18  | B8    | 1793 | ILE  | Mainchain         |
| 18  | B8    | 1794 | SER  | Mainchain         |
| 18  | B8    | 1797 | LEU  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B8    | 1798 | VAL  | Peptide           |
| 18  | B8    | 1799 | VAL  | Mainchain         |
| 18  | B8    | 1800 | ARG  | Mainchain         |
| 18  | B8    | 1801 | GLY  | Mainchain         |
| 18  | B8    | 1802 | ASP  | Mainchain         |
| 18  | B8    | 1803 | THR  | Mainchain         |
| 18  | B8    | 1804 | THR  | Mainchain         |
| 18  | B8    | 1806 | HIS  | Mainchain         |
| 18  | B8    | 1807 | PRO  | Mainchain         |
| 18  | B8    | 1808 | GLY  | Mainchain         |
| 18  | B8    | 1809 | SER  | Mainchain         |
| 18  | B8    | 192  | PRO  | Mainchain         |
| 18  | B8    | 2    | ALA  | Mainchain         |
| 18  | B8    | 249  | TYR  | Mainchain         |
| 18  | B8    | 298  | THR  | Mainchain         |
| 18  | B8    | 384  | ASP  | Mainchain         |
| 18  | B8    | 4    | PRO  | Mainchain         |
| 18  | B8    | 413  | ASP  | Mainchain         |
| 18  | B8    | 499  | ILE  | Mainchain         |
| 18  | B8    | 500  | THR  | Mainchain         |
| 18  | B8    | 504  | PRO  | Mainchain         |
| 18  | B8    | 505  | ALA  | Mainchain         |
| 18  | B8    | 506  | ASP  | Mainchain         |
| 18  | B8    | 508  | ALA  | Mainchain         |
| 18  | B8    | 606  | GLN  | Mainchain         |
| 18  | B8    | 608  | SER  | Mainchain         |
| 18  | B8    | 609  | TYR  | Mainchain         |
| 18  | B8    | 610  | VAL  | Mainchain         |
| 18  | B8    | 611  | ASN  | Mainchain         |
| 18  | B8    | 612  | GLY  | Mainchain         |
| 18  | B8    | 613  | LYS  | Mainchain         |
| 18  | B8    | 614  | MET  | Mainchain         |
| 18  | B8    | 617  | ASP  | Mainchain         |
| 18  | B8    | 671  | MET  | Mainchain         |
| 18  | B8    | 672  | THR  | Mainchain         |
| 18  | B8    | 673  | SER  | Mainchain         |
| 18  | B8    | 674  | CYS  | Mainchain         |
| 18  | B8    | 675  | SER  | Mainchain         |
| 18  | B8    | 676  | ASP  | Mainchain         |
| 18  | B8    | 677  | VAL  | Mainchain         |
| 18  | B8    | 679  | ASP  | Mainchain         |
| 18  | B8    | 681  | GLY  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 18  | B8    | 682  | TYR  | Mainchain         |
| 18  | B8    | 683  | ASN  | Mainchain         |
| 18  | B8    | 684  | ILE  | Mainchain         |
| 18  | B8    | 685  | SER  | Mainchain         |
| 18  | B8    | 688  | GLY  | Mainchain         |
| 18  | B8    | 689  | SER  | Mainchain         |
| 18  | B8    | 690  | TRP  | Mainchain         |
| 18  | B8    | 691  | SER  | Mainchain         |
| 18  | B8    | 693  | SER  | Mainchain         |
| 18  | B8    | 854  | SER  | Mainchain         |
| 18  | B8    | 855  | GLY  | Mainchain         |
| 18  | B8    | 907  | SER  | Mainchain         |
| 18  | B8    | 913  | SER  | Mainchain         |
| 18  | B8    | 914  | ASN  | Mainchain         |
| 18  | B8    | 915  | ALA  | Mainchain         |
| 18  | B8    | 969  | ASP  | Mainchain         |
| 18  | B8    | 970  | SER  | Mainchain         |
| 18  | B8    | 974  | SER  | Mainchain         |
| 18  | B8    | 975  | ASP  | Mainchain         |
| 18  | B8    | 976  | SER  | Mainchain         |
| 18  | B8    | 977  | SER  | Peptide,Mainchain |
| 18  | B8    | 978  | ASN  | Peptide,Mainchain |
| 18  | B8    | 979  | VAL  | Mainchain         |
| 18  | B8    | 980  | LYS  | Peptide,Mainchain |
| 18  | B8    | 981  | GLN  | Peptide,Mainchain |
| 18  | B8    | 982  | SER  | Peptide,Mainchain |
| 18  | B8    | 983  | ARG  | Mainchain         |
| 18  | B8    | 984  | LYS  | Peptide,Mainchain |
| 18  | B8    | 985  | ASP  | Peptide,Mainchain |
| 18  | B8    | 987  | SER  | Mainchain         |
| 18  | B8    | 988  | SER  | Mainchain         |
| 18  | B8    | 989  | ILE  | Mainchain         |
| 18  | B8    | 990  | PRO  | Mainchain         |
| 18  | B8    | 991  | ASP  | Mainchain         |
| 18  | B8    | 992  | TRP  | Mainchain         |
| 18  | B8    | 993  | ALA  | Mainchain         |
| 18  | B8    | 994  | CYS  | Mainchain         |
| 10  | C     | 1034 | SER  | Mainchain         |
| 10  | C     | 1037 | SER  | Mainchain         |
| 10  | C     | 105  | TRP  | Mainchain         |
| 10  | C     | 1052 | PHE  | Mainchain         |
| 10  | C     | 1053 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C     | 1054 | ARG  | Mainchain         |
| 10  | C     | 1055 | GLU  | Mainchain         |
| 10  | C     | 1056 | VAL  | Mainchain         |
| 10  | C     | 1058 | GLU  | Peptide,Mainchain |
| 10  | C     | 1059 | ALA  | Mainchain         |
| 10  | C     | 1060 | ALA  | Mainchain         |
| 10  | C     | 1061 | ASN  | Mainchain         |
| 10  | C     | 1062 | GLU  | Mainchain         |
| 10  | C     | 1063 | PRO  | Mainchain         |
| 10  | C     | 1064 | PHE  | Mainchain         |
| 10  | C     | 1065 | SER  | Mainchain         |
| 10  | C     | 1066 | SER  | Mainchain         |
| 10  | C     | 1067 | SER  | Peptide,Mainchain |
| 10  | C     | 1068 | THR  | Peptide,Mainchain |
| 10  | C     | 1069 | TYR  | Mainchain         |
| 10  | C     | 1071 | GLN  | Mainchain         |
| 10  | C     | 1072 | ASP  | Peptide,Mainchain |
| 10  | C     | 1074 | LEU  | Peptide,Mainchain |
| 10  | C     | 1075 | ASP  | Mainchain         |
| 10  | C     | 1077 | ALA  | Mainchain         |
| 10  | C     | 1078 | GLY  | Mainchain         |
| 10  | C     | 1079 | THR  | Mainchain         |
| 10  | C     | 1080 | SER  | Mainchain         |
| 10  | C     | 1081 | SER  | Mainchain         |
| 10  | C     | 1082 | ILE  | Mainchain         |
| 10  | C     | 1083 | SER  | Mainchain         |
| 10  | C     | 1084 | LYS  | Mainchain         |
| 10  | C     | 1111 | SER  | Mainchain         |
| 10  | C     | 1126 | ASP  | Mainchain         |
| 10  | C     | 1127 | THR  | Mainchain         |
| 10  | C     | 1128 | SER  | Peptide,Mainchain |
| 10  | C     | 1130 | SER  | Mainchain         |
| 10  | C     | 1161 | PHE  | Mainchain         |
| 10  | C     | 1162 | PRO  | Mainchain         |
| 10  | C     | 1163 | LEU  | Mainchain         |
| 10  | C     | 1166 | SER  | Mainchain         |
| 10  | C     | 1167 | PHE  | Mainchain         |
| 10  | C     | 1169 | ASN  | Mainchain         |
| 10  | C     | 1270 | SER  | Mainchain         |
| 10  | C     | 1272 | GLN  | Mainchain         |
| 10  | C     | 1273 | GLY  | Mainchain         |
| 10  | C     | 1274 | ALA  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C     | 1277 | SER  | Mainchain         |
| 10  | C     | 1280 | VAL  | Mainchain         |
| 10  | C     | 1287 | MET  | Mainchain         |
| 10  | C     | 1288 | VAL  | Mainchain         |
| 10  | C     | 1290 | HIS  | Mainchain         |
| 10  | C     | 1335 | ILE  | Mainchain         |
| 10  | C     | 1336 | ALA  | Mainchain         |
| 10  | C     | 1351 | GLU  | Mainchain         |
| 10  | C     | 1352 | GLN  | Peptide,Mainchain |
| 10  | C     | 1353 | ASP  | Mainchain         |
| 10  | C     | 1354 | GLY  | Mainchain         |
| 10  | C     | 1355 | GLU  | Mainchain         |
| 10  | C     | 1356 | ASP  | Mainchain         |
| 10  | C     | 1357 | LEU  | Mainchain         |
| 10  | C     | 1358 | ASP  | Mainchain         |
| 10  | C     | 1439 | ILE  | Mainchain         |
| 10  | C     | 1440 | SER  | Mainchain         |
| 10  | C     | 1443 | ASP  | Mainchain         |
| 10  | C     | 1445 | THR  | Mainchain         |
| 10  | C     | 1495 | SER  | Mainchain         |
| 10  | C     | 1496 | PHE  | Mainchain         |
| 10  | C     | 1497 | LYS  | Mainchain         |
| 10  | C     | 1498 | GLY  | Mainchain         |
| 10  | C     | 1499 | ASN  | Mainchain         |
| 10  | C     | 1503 | VAL  | Mainchain         |
| 10  | C     | 1504 | ASP  | Mainchain         |
| 10  | C     | 1505 | MET  | Mainchain         |
| 10  | C     | 1507 | LEU  | Mainchain         |
| 10  | C     | 1509 | SER  | Mainchain         |
| 10  | C     | 1536 | VAL  | Mainchain         |
| 10  | C     | 1617 | ALA  | Mainchain         |
| 10  | C     | 1618 | SER  | Mainchain         |
| 10  | C     | 1619 | PRO  | Mainchain         |
| 10  | C     | 1620 | ILE  | Mainchain         |
| 10  | C     | 1621 | LYS  | Peptide,Mainchain |
| 10  | C     | 1622 | SER  | Mainchain         |
| 10  | C     | 1623 | ILE  | Mainchain         |
| 10  | C     | 1624 | LEU  | Mainchain         |
| 10  | C     | 1625 | SER  | Mainchain         |
| 10  | C     | 1627 | GLY  | Mainchain         |
| 10  | C     | 1658 | ASP  | Mainchain         |
| 10  | C     | 1659 | ASP  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C     | 1660 | SER  | Mainchain         |
| 10  | C     | 1661 | LEU  | Mainchain         |
| 10  | C     | 1662 | ASP  | Peptide,Mainchain |
| 10  | C     | 1663 | SER  | Mainchain         |
| 10  | C     | 1666 | LYS  | Mainchain         |
| 10  | C     | 1667 | LEU  | Mainchain         |
| 10  | C     | 1772 | ASP  | Mainchain         |
| 10  | C     | 1776 | SER  | Mainchain         |
| 10  | C     | 1777 | SER  | Mainchain         |
| 10  | C     | 1778 | ASN  | Peptide,Mainchain |
| 10  | C     | 1779 | GLU  | Mainchain         |
| 10  | C     | 1780 | ARG  | Peptide,Mainchain |
| 10  | C     | 1781 | GLY  | Mainchain         |
| 10  | C     | 1782 | SER  | Mainchain         |
| 10  | C     | 1783 | TYR  | Mainchain         |
| 10  | C     | 187  | GLY  | Mainchain         |
| 10  | C     | 248  | LEU  | Mainchain         |
| 10  | C     | 250  | GLU  | Mainchain         |
| 10  | C     | 251  | GLY  | Mainchain         |
| 10  | C     | 280  | SER  | Mainchain         |
| 10  | C     | 282  | LYS  | Mainchain         |
| 10  | C     | 283  | SER  | Mainchain         |
| 10  | C     | 334  | MET  | Mainchain         |
| 10  | C     | 335  | ASP  | Peptide,Mainchain |
| 10  | C     | 336  | THR  | Peptide,Mainchain |
| 10  | C     | 337  | ILE  | Mainchain         |
| 10  | C     | 338  | SER  | Mainchain         |
| 10  | C     | 423  | SER  | Mainchain         |
| 10  | C     | 425  | PRO  | Mainchain         |
| 10  | C     | 426  | LEU  | Mainchain         |
| 10  | C     | 427  | ASP  | Mainchain         |
| 10  | C     | 428  | GLY  | Peptide,Mainchain |
| 10  | C     | 429  | SER  | Mainchain         |
| 10  | C     | 454  | SER  | Mainchain         |
| 10  | C     | 456  | ASN  | Mainchain         |
| 10  | C     | 530  | THR  | Mainchain         |
| 10  | C     | 533  | ALA  | Mainchain         |
| 10  | C     | 620  | PRO  | Mainchain         |
| 10  | C     | 621  | VAL  | Mainchain         |
| 10  | C     | 622  | VAL  | Mainchain         |
| 10  | C     | 623  | VAL  | Mainchain         |
| 10  | C     | 624  | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C     | 625  | SER  | Mainchain         |
| 10  | C     | 626  | GLN  | Mainchain         |
| 10  | C     | 627  | VAL  | Mainchain         |
| 10  | C     | 629  | LYS  | Mainchain         |
| 10  | C     | 631  | ASP  | Mainchain         |
| 10  | C     | 632  | GLN  | Mainchain         |
| 10  | C     | 633  | SER  | Mainchain         |
| 10  | C     | 634  | SER  | Mainchain         |
| 10  | C     | 635  | GLN  | Mainchain         |
| 10  | C     | 669  | GLY  | Peptide           |
| 10  | C     | 671  | LYS  | Peptide           |
| 10  | C     | 672  | ASP  | Mainchain         |
| 10  | C     | 673  | VAL  | Mainchain         |
| 10  | C     | 674  | ASN  | Mainchain         |
| 10  | C     | 675  | ASP  | Mainchain         |
| 10  | C     | 677  | GLY  | Mainchain         |
| 10  | C     | 716  | THR  | Mainchain         |
| 10  | C     | 717  | GLU  | Mainchain         |
| 10  | C     | 718  | HIS  | Mainchain         |
| 10  | C     | 719  | PRO  | Mainchain         |
| 10  | C     | 725  | LEU  | Mainchain         |
| 10  | C     | 727  | THR  | Mainchain         |
| 10  | C     | 728  | SER  | Mainchain         |
| 10  | C     | 729  | SER  | Mainchain         |
| 10  | C     | 849  | SER  | Mainchain         |
| 10  | C     | 881  | GLU  | Mainchain         |
| 10  | C16   | 1034 | SER  | Mainchain         |
| 10  | C16   | 1035 | GLY  | Mainchain         |
| 10  | C16   | 1037 | SER  | Mainchain         |
| 10  | C16   | 105  | TRP  | Mainchain         |
| 10  | C16   | 1052 | PHE  | Mainchain         |
| 10  | C16   | 1053 | GLY  | Mainchain         |
| 10  | C16   | 1054 | ARG  | Mainchain         |
| 10  | C16   | 1055 | GLU  | Mainchain         |
| 10  | C16   | 1056 | VAL  | Mainchain         |
| 10  | C16   | 1058 | GLU  | Peptide,Mainchain |
| 10  | C16   | 1059 | ALA  | Mainchain         |
| 10  | C16   | 1060 | ALA  | Mainchain         |
| 10  | C16   | 1061 | ASN  | Mainchain         |
| 10  | C16   | 1062 | GLU  | Mainchain         |
| 10  | C16   | 1063 | PRO  | Mainchain         |
| 10  | C16   | 1064 | PHE  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C16   | 1065 | SER  | Mainchain         |
| 10  | C16   | 1066 | SER  | Mainchain         |
| 10  | C16   | 1067 | SER  | Peptide,Mainchain |
| 10  | C16   | 1068 | THR  | Peptide,Mainchain |
| 10  | C16   | 1069 | TYR  | Mainchain         |
| 10  | C16   | 1071 | GLN  | Mainchain         |
| 10  | C16   | 1072 | ASP  | Peptide,Mainchain |
| 10  | C16   | 1074 | LEU  | Peptide,Mainchain |
| 10  | C16   | 1075 | ASP  | Mainchain         |
| 10  | C16   | 1077 | ALA  | Mainchain         |
| 10  | C16   | 1078 | GLY  | Mainchain         |
| 10  | C16   | 1079 | THR  | Mainchain         |
| 10  | C16   | 1080 | SER  | Mainchain         |
| 10  | C16   | 1081 | SER  | Mainchain         |
| 10  | C16   | 1082 | ILE  | Mainchain         |
| 10  | C16   | 1083 | SER  | Mainchain         |
| 10  | C16   | 1084 | LYS  | Mainchain         |
| 10  | C16   | 1111 | SER  | Mainchain         |
| 10  | C16   | 1126 | ASP  | Mainchain         |
| 10  | C16   | 1127 | THR  | Mainchain         |
| 10  | C16   | 1128 | SER  | Peptide,Mainchain |
| 10  | C16   | 1130 | SER  | Mainchain         |
| 10  | C16   | 1161 | PHE  | Mainchain         |
| 10  | C16   | 1162 | PRO  | Mainchain         |
| 10  | C16   | 1163 | LEU  | Mainchain         |
| 10  | C16   | 1166 | SER  | Mainchain         |
| 10  | C16   | 1167 | PHE  | Mainchain         |
| 10  | C16   | 1169 | ASN  | Mainchain         |
| 10  | C16   | 1270 | SER  | Mainchain         |
| 10  | C16   | 1272 | GLN  | Mainchain         |
| 10  | C16   | 1273 | GLY  | Mainchain         |
| 10  | C16   | 1274 | ALA  | Mainchain         |
| 10  | C16   | 1277 | SER  | Mainchain         |
| 10  | C16   | 1280 | VAL  | Mainchain         |
| 10  | C16   | 1287 | MET  | Mainchain         |
| 10  | C16   | 1288 | VAL  | Mainchain         |
| 10  | C16   | 1290 | HIS  | Mainchain         |
| 10  | C16   | 1335 | ILE  | Mainchain         |
| 10  | C16   | 1336 | ALA  | Mainchain         |
| 10  | C16   | 1351 | GLU  | Mainchain         |
| 10  | C16   | 1352 | GLN  | Peptide,Mainchain |
| 10  | C16   | 1353 | ASP  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C16   | 1354 | GLY  | Mainchain         |
| 10  | C16   | 1355 | GLU  | Mainchain         |
| 10  | C16   | 1356 | ASP  | Mainchain         |
| 10  | C16   | 1357 | LEU  | Mainchain         |
| 10  | C16   | 1358 | ASP  | Mainchain         |
| 10  | C16   | 1439 | ILE  | Mainchain         |
| 10  | C16   | 1440 | SER  | Mainchain         |
| 10  | C16   | 1443 | ASP  | Mainchain         |
| 10  | C16   | 1445 | THR  | Mainchain         |
| 10  | C16   | 1495 | SER  | Mainchain         |
| 10  | C16   | 1496 | PHE  | Mainchain         |
| 10  | C16   | 1497 | LYS  | Mainchain         |
| 10  | C16   | 1498 | GLY  | Mainchain         |
| 10  | C16   | 1499 | ASN  | Mainchain         |
| 10  | C16   | 1503 | VAL  | Mainchain         |
| 10  | C16   | 1504 | ASP  | Mainchain         |
| 10  | C16   | 1505 | MET  | Mainchain         |
| 10  | C16   | 1507 | LEU  | Mainchain         |
| 10  | C16   | 1509 | SER  | Mainchain         |
| 10  | C16   | 1536 | VAL  | Mainchain         |
| 10  | C16   | 1540 | GLU  | Mainchain         |
| 10  | C16   | 1541 | PHE  | Mainchain         |
| 10  | C16   | 1542 | PHE  | Mainchain         |
| 10  | C16   | 1543 | GLU  | Mainchain         |
| 10  | C16   | 1544 | GLY  | Mainchain         |
| 10  | C16   | 1617 | ALA  | Mainchain         |
| 10  | C16   | 1618 | SER  | Mainchain         |
| 10  | C16   | 1619 | PRO  | Mainchain         |
| 10  | C16   | 1620 | ILE  | Mainchain         |
| 10  | C16   | 1621 | LYS  | Peptide,Mainchain |
| 10  | C16   | 1622 | SER  | Mainchain         |
| 10  | C16   | 1623 | ILE  | Mainchain         |
| 10  | C16   | 1624 | LEU  | Mainchain         |
| 10  | C16   | 1625 | SER  | Mainchain         |
| 10  | C16   | 1627 | GLY  | Mainchain         |
| 10  | C16   | 1658 | ASP  | Mainchain         |
| 10  | C16   | 1659 | ASP  | Mainchain         |
| 10  | C16   | 1660 | SER  | Mainchain         |
| 10  | C16   | 1661 | LEU  | Mainchain         |
| 10  | C16   | 1662 | ASP  | Peptide,Mainchain |
| 10  | C16   | 1663 | SER  | Mainchain         |
| 10  | C16   | 1666 | LYS  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C16   | 1667 | LEU  | Mainchain         |
| 10  | C16   | 1772 | ASP  | Mainchain         |
| 10  | C16   | 1776 | SER  | Mainchain         |
| 10  | C16   | 1777 | SER  | Mainchain         |
| 10  | C16   | 1778 | ASN  | Peptide,Mainchain |
| 10  | C16   | 1779 | GLU  | Mainchain         |
| 10  | C16   | 1780 | ARG  | Peptide,Mainchain |
| 10  | C16   | 1781 | GLY  | Mainchain         |
| 10  | C16   | 1782 | SER  | Mainchain         |
| 10  | C16   | 1783 | TYR  | Mainchain         |
| 10  | C16   | 187  | GLY  | Mainchain         |
| 10  | C16   | 248  | LEU  | Mainchain         |
| 10  | C16   | 250  | GLU  | Mainchain         |
| 10  | C16   | 251  | GLY  | Mainchain         |
| 10  | C16   | 280  | SER  | Mainchain         |
| 10  | C16   | 282  | LYS  | Mainchain         |
| 10  | C16   | 283  | SER  | Mainchain         |
| 10  | C16   | 334  | MET  | Mainchain         |
| 10  | C16   | 335  | ASP  | Peptide,Mainchain |
| 10  | C16   | 336  | THR  | Peptide,Mainchain |
| 10  | C16   | 337  | ILE  | Mainchain         |
| 10  | C16   | 338  | SER  | Mainchain         |
| 10  | C16   | 423  | SER  | Mainchain         |
| 10  | C16   | 425  | PRO  | Mainchain         |
| 10  | C16   | 426  | LEU  | Mainchain         |
| 10  | C16   | 427  | ASP  | Mainchain         |
| 10  | C16   | 428  | GLY  | Peptide,Mainchain |
| 10  | C16   | 429  | SER  | Mainchain         |
| 10  | C16   | 447  | PHE  | Mainchain         |
| 10  | C16   | 454  | SER  | Mainchain         |
| 10  | C16   | 456  | ASN  | Mainchain         |
| 10  | C16   | 530  | THR  | Mainchain         |
| 10  | C16   | 533  | ALA  | Mainchain         |
| 10  | C16   | 620  | PRO  | Mainchain         |
| 10  | C16   | 621  | VAL  | Mainchain         |
| 10  | C16   | 622  | VAL  | Mainchain         |
| 10  | C16   | 623  | VAL  | Mainchain         |
| 10  | C16   | 624  | GLY  | Mainchain         |
| 10  | C16   | 625  | SER  | Mainchain         |
| 10  | C16   | 626  | GLN  | Mainchain         |
| 10  | C16   | 627  | VAL  | Mainchain         |
| 10  | C16   | 629  | LYS  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C16   | 631  | ASP  | Mainchain         |
| 10  | C16   | 632  | GLN  | Mainchain         |
| 10  | C16   | 633  | SER  | Mainchain         |
| 10  | C16   | 634  | SER  | Mainchain         |
| 10  | C16   | 635  | GLN  | Mainchain         |
| 10  | C16   | 669  | GLY  | Peptide           |
| 10  | C16   | 671  | LYS  | Peptide           |
| 10  | C16   | 672  | ASP  | Mainchain         |
| 10  | C16   | 673  | VAL  | Mainchain         |
| 10  | C16   | 674  | ASN  | Mainchain         |
| 10  | C16   | 675  | ASP  | Mainchain         |
| 10  | C16   | 677  | GLY  | Mainchain         |
| 10  | C16   | 716  | THR  | Mainchain         |
| 10  | C16   | 717  | GLU  | Mainchain         |
| 10  | C16   | 718  | HIS  | Mainchain         |
| 10  | C16   | 719  | PRO  | Mainchain         |
| 10  | C16   | 725  | LEU  | Mainchain         |
| 10  | C16   | 727  | THR  | Mainchain         |
| 10  | C16   | 728  | SER  | Mainchain         |
| 10  | C16   | 729  | SER  | Mainchain         |
| 10  | C16   | 849  | SER  | Mainchain         |
| 10  | C16   | 881  | GLU  | Mainchain         |
| 10  | C24   | 1034 | SER  | Mainchain         |
| 10  | C24   | 1035 | GLY  | Mainchain         |
| 10  | C24   | 1037 | SER  | Mainchain         |
| 10  | C24   | 105  | TRP  | Mainchain         |
| 10  | C24   | 1052 | PHE  | Mainchain         |
| 10  | C24   | 1053 | GLY  | Mainchain         |
| 10  | C24   | 1054 | ARG  | Mainchain         |
| 10  | C24   | 1055 | GLU  | Mainchain         |
| 10  | C24   | 1056 | VAL  | Mainchain         |
| 10  | C24   | 1058 | GLU  | Peptide,Mainchain |
| 10  | C24   | 1059 | ALA  | Mainchain         |
| 10  | C24   | 1060 | ALA  | Mainchain         |
| 10  | C24   | 1061 | ASN  | Mainchain         |
| 10  | C24   | 1062 | GLU  | Mainchain         |
| 10  | C24   | 1063 | PRO  | Mainchain         |
| 10  | C24   | 1064 | PHE  | Mainchain         |
| 10  | C24   | 1065 | SER  | Mainchain         |
| 10  | C24   | 1066 | SER  | Mainchain         |
| 10  | C24   | 1067 | SER  | Peptide,Mainchain |
| 10  | C24   | 1068 | THR  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C24   | 1069 | TYR  | Mainchain         |
| 10  | C24   | 1071 | GLN  | Mainchain         |
| 10  | C24   | 1072 | ASP  | Peptide,Mainchain |
| 10  | C24   | 1074 | LEU  | Peptide,Mainchain |
| 10  | C24   | 1075 | ASP  | Mainchain         |
| 10  | C24   | 1077 | ALA  | Mainchain         |
| 10  | C24   | 1078 | GLY  | Mainchain         |
| 10  | C24   | 1079 | THR  | Mainchain         |
| 10  | C24   | 1080 | SER  | Mainchain         |
| 10  | C24   | 1081 | SER  | Mainchain         |
| 10  | C24   | 1082 | ILE  | Mainchain         |
| 10  | C24   | 1083 | SER  | Mainchain         |
| 10  | C24   | 1084 | LYS  | Mainchain         |
| 10  | C24   | 1111 | SER  | Mainchain         |
| 10  | C24   | 1126 | ASP  | Mainchain         |
| 10  | C24   | 1127 | THR  | Mainchain         |
| 10  | C24   | 1128 | SER  | Peptide,Mainchain |
| 10  | C24   | 1130 | SER  | Mainchain         |
| 10  | C24   | 1161 | PHE  | Mainchain         |
| 10  | C24   | 1162 | PRO  | Mainchain         |
| 10  | C24   | 1163 | LEU  | Mainchain         |
| 10  | C24   | 1166 | SER  | Mainchain         |
| 10  | C24   | 1167 | PHE  | Mainchain         |
| 10  | C24   | 1169 | ASN  | Mainchain         |
| 10  | C24   | 1270 | SER  | Mainchain         |
| 10  | C24   | 1272 | GLN  | Mainchain         |
| 10  | C24   | 1273 | GLY  | Mainchain         |
| 10  | C24   | 1274 | ALA  | Mainchain         |
| 10  | C24   | 1277 | SER  | Mainchain         |
| 10  | C24   | 1280 | VAL  | Mainchain         |
| 10  | C24   | 1287 | MET  | Mainchain         |
| 10  | C24   | 1288 | VAL  | Mainchain         |
| 10  | C24   | 1290 | HIS  | Mainchain         |
| 10  | C24   | 1335 | ILE  | Mainchain         |
| 10  | C24   | 1336 | ALA  | Mainchain         |
| 10  | C24   | 1351 | GLU  | Mainchain         |
| 10  | C24   | 1352 | GLN  | Peptide,Mainchain |
| 10  | C24   | 1353 | ASP  | Mainchain         |
| 10  | C24   | 1354 | GLY  | Mainchain         |
| 10  | C24   | 1355 | GLU  | Mainchain         |
| 10  | C24   | 1356 | ASP  | Mainchain         |
| 10  | C24   | 1357 | LEU  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C24   | 1358 | ASP  | Mainchain         |
| 10  | C24   | 1439 | ILE  | Mainchain         |
| 10  | C24   | 1440 | SER  | Mainchain         |
| 10  | C24   | 1443 | ASP  | Mainchain         |
| 10  | C24   | 1445 | THR  | Mainchain         |
| 10  | C24   | 1495 | SER  | Mainchain         |
| 10  | C24   | 1496 | PHE  | Mainchain         |
| 10  | C24   | 1497 | LYS  | Mainchain         |
| 10  | C24   | 1498 | GLY  | Mainchain         |
| 10  | C24   | 1499 | ASN  | Mainchain         |
| 10  | C24   | 1503 | VAL  | Mainchain         |
| 10  | C24   | 1504 | ASP  | Mainchain         |
| 10  | C24   | 1505 | MET  | Mainchain         |
| 10  | C24   | 1507 | LEU  | Mainchain         |
| 10  | C24   | 1509 | SER  | Mainchain         |
| 10  | C24   | 1536 | VAL  | Mainchain         |
| 10  | C24   | 1540 | GLU  | Mainchain         |
| 10  | C24   | 1541 | PHE  | Mainchain         |
| 10  | C24   | 1542 | PHE  | Mainchain         |
| 10  | C24   | 1543 | GLU  | Mainchain         |
| 10  | C24   | 1544 | GLY  | Mainchain         |
| 10  | C24   | 1617 | ALA  | Mainchain         |
| 10  | C24   | 1618 | SER  | Mainchain         |
| 10  | C24   | 1619 | PRO  | Mainchain         |
| 10  | C24   | 1620 | ILE  | Mainchain         |
| 10  | C24   | 1621 | LYS  | Peptide,Mainchain |
| 10  | C24   | 1622 | SER  | Mainchain         |
| 10  | C24   | 1623 | ILE  | Mainchain         |
| 10  | C24   | 1624 | LEU  | Mainchain         |
| 10  | C24   | 1625 | SER  | Mainchain         |
| 10  | C24   | 1627 | GLY  | Mainchain         |
| 10  | C24   | 1658 | ASP  | Mainchain         |
| 10  | C24   | 1659 | ASP  | Mainchain         |
| 10  | C24   | 1660 | SER  | Mainchain         |
| 10  | C24   | 1661 | LEU  | Mainchain         |
| 10  | C24   | 1662 | ASP  | Peptide,Mainchain |
| 10  | C24   | 1663 | SER  | Mainchain         |
| 10  | C24   | 1666 | LYS  | Mainchain         |
| 10  | C24   | 1667 | LEU  | Mainchain         |
| 10  | C24   | 1772 | ASP  | Mainchain         |
| 10  | C24   | 1776 | SER  | Mainchain         |
| 10  | C24   | 1777 | SER  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C24   | 1778 | ASN  | Peptide,Mainchain |
| 10  | C24   | 1779 | GLU  | Mainchain         |
| 10  | C24   | 1780 | ARG  | Peptide,Mainchain |
| 10  | C24   | 1781 | GLY  | Mainchain         |
| 10  | C24   | 1782 | SER  | Mainchain         |
| 10  | C24   | 1783 | TYR  | Mainchain         |
| 10  | C24   | 187  | GLY  | Mainchain         |
| 10  | C24   | 248  | LEU  | Mainchain         |
| 10  | C24   | 250  | GLU  | Mainchain         |
| 10  | C24   | 251  | GLY  | Mainchain         |
| 10  | C24   | 280  | SER  | Mainchain         |
| 10  | C24   | 282  | LYS  | Mainchain         |
| 10  | C24   | 283  | SER  | Mainchain         |
| 10  | C24   | 334  | MET  | Mainchain         |
| 10  | C24   | 335  | ASP  | Peptide,Mainchain |
| 10  | C24   | 336  | THR  | Peptide,Mainchain |
| 10  | C24   | 337  | ILE  | Mainchain         |
| 10  | C24   | 338  | SER  | Mainchain         |
| 10  | C24   | 423  | SER  | Mainchain         |
| 10  | C24   | 425  | PRO  | Mainchain         |
| 10  | C24   | 426  | LEU  | Mainchain         |
| 10  | C24   | 427  | ASP  | Mainchain         |
| 10  | C24   | 428  | GLY  | Peptide,Mainchain |
| 10  | C24   | 429  | SER  | Mainchain         |
| 10  | C24   | 447  | PHE  | Mainchain         |
| 10  | C24   | 454  | SER  | Mainchain         |
| 10  | C24   | 456  | ASN  | Mainchain         |
| 10  | C24   | 530  | THR  | Mainchain         |
| 10  | C24   | 533  | ALA  | Mainchain         |
| 10  | C24   | 620  | PRO  | Mainchain         |
| 10  | C24   | 621  | VAL  | Mainchain         |
| 10  | C24   | 622  | VAL  | Mainchain         |
| 10  | C24   | 623  | VAL  | Mainchain         |
| 10  | C24   | 624  | GLY  | Mainchain         |
| 10  | C24   | 625  | SER  | Mainchain         |
| 10  | C24   | 626  | GLN  | Mainchain         |
| 10  | C24   | 627  | VAL  | Mainchain         |
| 10  | C24   | 629  | LYS  | Mainchain         |
| 10  | C24   | 631  | ASP  | Mainchain         |
| 10  | C24   | 632  | GLN  | Mainchain         |
| 10  | C24   | 633  | SER  | Mainchain         |
| 10  | C24   | 634  | SER  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C24   | 635  | GLN  | Mainchain         |
| 10  | C24   | 669  | GLY  | Peptide           |
| 10  | C24   | 671  | LYS  | Peptide           |
| 10  | C24   | 672  | ASP  | Mainchain         |
| 10  | C24   | 673  | VAL  | Mainchain         |
| 10  | C24   | 674  | ASN  | Mainchain         |
| 10  | C24   | 675  | ASP  | Mainchain         |
| 10  | C24   | 677  | GLY  | Mainchain         |
| 10  | C24   | 716  | THR  | Mainchain         |
| 10  | C24   | 717  | GLU  | Mainchain         |
| 10  | C24   | 718  | HIS  | Mainchain         |
| 10  | C24   | 719  | PRO  | Mainchain         |
| 10  | C24   | 725  | LEU  | Mainchain         |
| 10  | C24   | 727  | THR  | Mainchain         |
| 10  | C24   | 728  | SER  | Mainchain         |
| 10  | C24   | 729  | SER  | Mainchain         |
| 10  | C24   | 849  | SER  | Mainchain         |
| 10  | C24   | 881  | GLU  | Mainchain         |
| 10  | C32   | 1034 | SER  | Mainchain         |
| 10  | C32   | 1035 | GLY  | Mainchain         |
| 10  | C32   | 1037 | SER  | Mainchain         |
| 10  | C32   | 105  | TRP  | Mainchain         |
| 10  | C32   | 1052 | PHE  | Mainchain         |
| 10  | C32   | 1053 | GLY  | Mainchain         |
| 10  | C32   | 1054 | ARG  | Mainchain         |
| 10  | C32   | 1055 | GLU  | Mainchain         |
| 10  | C32   | 1056 | VAL  | Mainchain         |
| 10  | C32   | 1058 | GLU  | Peptide,Mainchain |
| 10  | C32   | 1059 | ALA  | Mainchain         |
| 10  | C32   | 1060 | ALA  | Mainchain         |
| 10  | C32   | 1061 | ASN  | Mainchain         |
| 10  | C32   | 1062 | GLU  | Mainchain         |
| 10  | C32   | 1063 | PRO  | Mainchain         |
| 10  | C32   | 1064 | PHE  | Mainchain         |
| 10  | C32   | 1065 | SER  | Mainchain         |
| 10  | C32   | 1066 | SER  | Mainchain         |
| 10  | C32   | 1067 | SER  | Peptide,Mainchain |
| 10  | C32   | 1068 | THR  | Peptide,Mainchain |
| 10  | C32   | 1069 | TYR  | Mainchain         |
| 10  | C32   | 1071 | GLN  | Mainchain         |
| 10  | C32   | 1072 | ASP  | Peptide,Mainchain |
| 10  | C32   | 1074 | LEU  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C32   | 1075 | ASP  | Mainchain         |
| 10  | C32   | 1077 | ALA  | Mainchain         |
| 10  | C32   | 1078 | GLY  | Mainchain         |
| 10  | C32   | 1079 | THR  | Mainchain         |
| 10  | C32   | 1080 | SER  | Mainchain         |
| 10  | C32   | 1081 | SER  | Mainchain         |
| 10  | C32   | 1082 | ILE  | Mainchain         |
| 10  | C32   | 1083 | SER  | Mainchain         |
| 10  | C32   | 1084 | LYS  | Mainchain         |
| 10  | C32   | 1111 | SER  | Mainchain         |
| 10  | C32   | 1126 | ASP  | Mainchain         |
| 10  | C32   | 1127 | THR  | Mainchain         |
| 10  | C32   | 1128 | SER  | Peptide,Mainchain |
| 10  | C32   | 1130 | SER  | Mainchain         |
| 10  | C32   | 1161 | PHE  | Mainchain         |
| 10  | C32   | 1162 | PRO  | Mainchain         |
| 10  | C32   | 1163 | LEU  | Mainchain         |
| 10  | C32   | 1166 | SER  | Mainchain         |
| 10  | C32   | 1167 | PHE  | Mainchain         |
| 10  | C32   | 1169 | ASN  | Mainchain         |
| 10  | C32   | 1270 | SER  | Mainchain         |
| 10  | C32   | 1272 | GLN  | Mainchain         |
| 10  | C32   | 1273 | GLY  | Mainchain         |
| 10  | C32   | 1274 | ALA  | Mainchain         |
| 10  | C32   | 1277 | SER  | Mainchain         |
| 10  | C32   | 1280 | VAL  | Mainchain         |
| 10  | C32   | 1287 | MET  | Mainchain         |
| 10  | C32   | 1288 | VAL  | Mainchain         |
| 10  | C32   | 1290 | HIS  | Mainchain         |
| 10  | C32   | 1335 | ILE  | Mainchain         |
| 10  | C32   | 1336 | ALA  | Mainchain         |
| 10  | C32   | 1351 | GLU  | Mainchain         |
| 10  | C32   | 1352 | GLN  | Peptide,Mainchain |
| 10  | C32   | 1353 | ASP  | Mainchain         |
| 10  | C32   | 1354 | GLY  | Mainchain         |
| 10  | C32   | 1355 | GLU  | Mainchain         |
| 10  | C32   | 1356 | ASP  | Mainchain         |
| 10  | C32   | 1357 | LEU  | Mainchain         |
| 10  | C32   | 1358 | ASP  | Mainchain         |
| 10  | C32   | 1439 | ILE  | Mainchain         |
| 10  | C32   | 1440 | SER  | Mainchain         |
| 10  | C32   | 1443 | ASP  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C32   | 1445 | THR  | Mainchain         |
| 10  | C32   | 1495 | SER  | Mainchain         |
| 10  | C32   | 1496 | PHE  | Mainchain         |
| 10  | C32   | 1497 | LYS  | Mainchain         |
| 10  | C32   | 1498 | GLY  | Mainchain         |
| 10  | C32   | 1499 | ASN  | Mainchain         |
| 10  | C32   | 1503 | VAL  | Mainchain         |
| 10  | C32   | 1504 | ASP  | Mainchain         |
| 10  | C32   | 1505 | MET  | Mainchain         |
| 10  | C32   | 1507 | LEU  | Mainchain         |
| 10  | C32   | 1509 | SER  | Mainchain         |
| 10  | C32   | 1536 | VAL  | Mainchain         |
| 10  | C32   | 1540 | GLU  | Mainchain         |
| 10  | C32   | 1541 | PHE  | Mainchain         |
| 10  | C32   | 1542 | PHE  | Mainchain         |
| 10  | C32   | 1543 | GLU  | Mainchain         |
| 10  | C32   | 1544 | GLY  | Mainchain         |
| 10  | C32   | 1617 | ALA  | Mainchain         |
| 10  | C32   | 1618 | SER  | Mainchain         |
| 10  | C32   | 1619 | PRO  | Mainchain         |
| 10  | C32   | 1620 | ILE  | Mainchain         |
| 10  | C32   | 1621 | LYS  | Peptide,Mainchain |
| 10  | C32   | 1622 | SER  | Mainchain         |
| 10  | C32   | 1623 | ILE  | Mainchain         |
| 10  | C32   | 1624 | LEU  | Mainchain         |
| 10  | C32   | 1625 | SER  | Mainchain         |
| 10  | C32   | 1627 | GLY  | Mainchain         |
| 10  | C32   | 1658 | ASP  | Mainchain         |
| 10  | C32   | 1659 | ASP  | Mainchain         |
| 10  | C32   | 1660 | SER  | Mainchain         |
| 10  | C32   | 1661 | LEU  | Mainchain         |
| 10  | C32   | 1662 | ASP  | Peptide,Mainchain |
| 10  | C32   | 1663 | SER  | Mainchain         |
| 10  | C32   | 1666 | LYS  | Mainchain         |
| 10  | C32   | 1667 | LEU  | Mainchain         |
| 10  | C32   | 1772 | ASP  | Mainchain         |
| 10  | C32   | 1776 | SER  | Mainchain         |
| 10  | C32   | 1777 | SER  | Mainchain         |
| 10  | C32   | 1778 | ASN  | Peptide,Mainchain |
| 10  | C32   | 1779 | GLU  | Mainchain         |
| 10  | C32   | 1780 | ARG  | Peptide,Mainchain |
| 10  | C32   | 1781 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C32   | 1782 | SER  | Mainchain         |
| 10  | C32   | 1783 | TYR  | Mainchain         |
| 10  | C32   | 187  | GLY  | Mainchain         |
| 10  | C32   | 248  | LEU  | Mainchain         |
| 10  | C32   | 250  | GLU  | Mainchain         |
| 10  | C32   | 251  | GLY  | Mainchain         |
| 10  | C32   | 280  | SER  | Mainchain         |
| 10  | C32   | 282  | LYS  | Mainchain         |
| 10  | C32   | 283  | SER  | Mainchain         |
| 10  | C32   | 334  | MET  | Mainchain         |
| 10  | C32   | 335  | ASP  | Peptide,Mainchain |
| 10  | C32   | 336  | THR  | Peptide,Mainchain |
| 10  | C32   | 337  | ILE  | Mainchain         |
| 10  | C32   | 338  | SER  | Mainchain         |
| 10  | C32   | 423  | SER  | Mainchain         |
| 10  | C32   | 425  | PRO  | Mainchain         |
| 10  | C32   | 426  | LEU  | Mainchain         |
| 10  | C32   | 427  | ASP  | Mainchain         |
| 10  | C32   | 428  | GLY  | Peptide,Mainchain |
| 10  | C32   | 429  | SER  | Mainchain         |
| 10  | C32   | 447  | PHE  | Mainchain         |
| 10  | C32   | 454  | SER  | Mainchain         |
| 10  | C32   | 456  | ASN  | Mainchain         |
| 10  | C32   | 530  | THR  | Mainchain         |
| 10  | C32   | 533  | ALA  | Mainchain         |
| 10  | C32   | 620  | PRO  | Mainchain         |
| 10  | C32   | 621  | VAL  | Mainchain         |
| 10  | C32   | 622  | VAL  | Mainchain         |
| 10  | C32   | 623  | VAL  | Mainchain         |
| 10  | C32   | 624  | GLY  | Mainchain         |
| 10  | C32   | 625  | SER  | Mainchain         |
| 10  | C32   | 626  | GLN  | Mainchain         |
| 10  | C32   | 627  | VAL  | Mainchain         |
| 10  | C32   | 629  | LYS  | Mainchain         |
| 10  | C32   | 631  | ASP  | Mainchain         |
| 10  | C32   | 632  | GLN  | Mainchain         |
| 10  | C32   | 633  | SER  | Mainchain         |
| 10  | C32   | 634  | SER  | Mainchain         |
| 10  | C32   | 635  | GLN  | Mainchain         |
| 10  | C32   | 669  | GLY  | Peptide           |
| 10  | C32   | 671  | LYS  | Peptide           |
| 10  | C32   | 672  | ASP  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C32   | 673  | VAL  | Mainchain         |
| 10  | C32   | 674  | ASN  | Mainchain         |
| 10  | C32   | 675  | ASP  | Mainchain         |
| 10  | C32   | 677  | GLY  | Mainchain         |
| 10  | C32   | 716  | THR  | Mainchain         |
| 10  | C32   | 717  | GLU  | Mainchain         |
| 10  | C32   | 718  | HIS  | Mainchain         |
| 10  | C32   | 719  | PRO  | Mainchain         |
| 10  | C32   | 725  | LEU  | Mainchain         |
| 10  | C32   | 727  | THR  | Mainchain         |
| 10  | C32   | 728  | SER  | Mainchain         |
| 10  | C32   | 729  | SER  | Mainchain         |
| 10  | C32   | 849  | SER  | Mainchain         |
| 10  | C32   | 881  | GLU  | Mainchain         |
| 10  | C8    | 1034 | SER  | Mainchain         |
| 10  | C8    | 1037 | SER  | Mainchain         |
| 10  | C8    | 105  | TRP  | Mainchain         |
| 10  | C8    | 1052 | PHE  | Mainchain         |
| 10  | C8    | 1053 | GLY  | Mainchain         |
| 10  | C8    | 1054 | ARG  | Mainchain         |
| 10  | C8    | 1055 | GLU  | Mainchain         |
| 10  | C8    | 1056 | VAL  | Mainchain         |
| 10  | C8    | 1058 | GLU  | Peptide,Mainchain |
| 10  | C8    | 1059 | ALA  | Mainchain         |
| 10  | C8    | 1060 | ALA  | Mainchain         |
| 10  | C8    | 1061 | ASN  | Mainchain         |
| 10  | C8    | 1062 | GLU  | Mainchain         |
| 10  | C8    | 1063 | PRO  | Mainchain         |
| 10  | C8    | 1064 | PHE  | Mainchain         |
| 10  | C8    | 1065 | SER  | Mainchain         |
| 10  | C8    | 1066 | SER  | Mainchain         |
| 10  | C8    | 1067 | SER  | Peptide,Mainchain |
| 10  | C8    | 1068 | THR  | Peptide,Mainchain |
| 10  | C8    | 1069 | TYR  | Mainchain         |
| 10  | C8    | 1071 | GLN  | Mainchain         |
| 10  | C8    | 1072 | ASP  | Peptide,Mainchain |
| 10  | C8    | 1074 | LEU  | Peptide,Mainchain |
| 10  | C8    | 1075 | ASP  | Mainchain         |
| 10  | C8    | 1077 | ALA  | Mainchain         |
| 10  | C8    | 1078 | GLY  | Mainchain         |
| 10  | C8    | 1079 | THR  | Mainchain         |
| 10  | C8    | 1080 | SER  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C8    | 1081 | SER  | Mainchain         |
| 10  | C8    | 1082 | ILE  | Mainchain         |
| 10  | C8    | 1083 | SER  | Mainchain         |
| 10  | C8    | 1084 | LYS  | Mainchain         |
| 10  | C8    | 1111 | SER  | Mainchain         |
| 10  | C8    | 1126 | ASP  | Mainchain         |
| 10  | C8    | 1127 | THR  | Mainchain         |
| 10  | C8    | 1128 | SER  | Peptide,Mainchain |
| 10  | C8    | 1130 | SER  | Mainchain         |
| 10  | C8    | 1161 | PHE  | Mainchain         |
| 10  | C8    | 1162 | PRO  | Mainchain         |
| 10  | C8    | 1163 | LEU  | Mainchain         |
| 10  | C8    | 1166 | SER  | Mainchain         |
| 10  | C8    | 1167 | PHE  | Mainchain         |
| 10  | C8    | 1169 | ASN  | Mainchain         |
| 10  | C8    | 1270 | SER  | Mainchain         |
| 10  | C8    | 1272 | GLN  | Mainchain         |
| 10  | C8    | 1273 | GLY  | Mainchain         |
| 10  | C8    | 1274 | ALA  | Mainchain         |
| 10  | C8    | 1277 | SER  | Mainchain         |
| 10  | C8    | 1280 | VAL  | Mainchain         |
| 10  | C8    | 1287 | MET  | Mainchain         |
| 10  | C8    | 1288 | VAL  | Mainchain         |
| 10  | C8    | 1290 | HIS  | Mainchain         |
| 10  | C8    | 1335 | ILE  | Mainchain         |
| 10  | C8    | 1336 | ALA  | Mainchain         |
| 10  | C8    | 1351 | GLU  | Mainchain         |
| 10  | C8    | 1352 | GLN  | Peptide,Mainchain |
| 10  | C8    | 1353 | ASP  | Mainchain         |
| 10  | C8    | 1354 | GLY  | Mainchain         |
| 10  | C8    | 1355 | GLU  | Mainchain         |
| 10  | C8    | 1356 | ASP  | Mainchain         |
| 10  | C8    | 1357 | LEU  | Mainchain         |
| 10  | C8    | 1358 | ASP  | Mainchain         |
| 10  | C8    | 1439 | ILE  | Mainchain         |
| 10  | C8    | 1440 | SER  | Mainchain         |
| 10  | C8    | 1443 | ASP  | Mainchain         |
| 10  | C8    | 1445 | THR  | Mainchain         |
| 10  | C8    | 1495 | SER  | Mainchain         |
| 10  | C8    | 1496 | PHE  | Mainchain         |
| 10  | C8    | 1497 | LYS  | Mainchain         |
| 10  | C8    | 1498 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C8    | 1499 | ASN  | Mainchain         |
| 10  | C8    | 1503 | VAL  | Mainchain         |
| 10  | C8    | 1504 | ASP  | Mainchain         |
| 10  | C8    | 1505 | MET  | Mainchain         |
| 10  | C8    | 1507 | LEU  | Mainchain         |
| 10  | C8    | 1509 | SER  | Mainchain         |
| 10  | C8    | 1536 | VAL  | Mainchain         |
| 10  | C8    | 1540 | GLU  | Mainchain         |
| 10  | C8    | 1541 | PHE  | Mainchain         |
| 10  | C8    | 1542 | PHE  | Mainchain         |
| 10  | C8    | 1543 | GLU  | Mainchain         |
| 10  | C8    | 1544 | GLY  | Mainchain         |
| 10  | C8    | 1617 | ALA  | Mainchain         |
| 10  | C8    | 1618 | SER  | Mainchain         |
| 10  | C8    | 1619 | PRO  | Mainchain         |
| 10  | C8    | 1620 | ILE  | Mainchain         |
| 10  | C8    | 1621 | LYS  | Peptide,Mainchain |
| 10  | C8    | 1622 | SER  | Mainchain         |
| 10  | C8    | 1623 | ILE  | Mainchain         |
| 10  | C8    | 1624 | LEU  | Mainchain         |
| 10  | C8    | 1625 | SER  | Mainchain         |
| 10  | C8    | 1627 | GLY  | Mainchain         |
| 10  | C8    | 1772 | ASP  | Mainchain         |
| 10  | C8    | 1776 | SER  | Mainchain         |
| 10  | C8    | 1777 | SER  | Mainchain         |
| 10  | C8    | 1778 | ASN  | Peptide,Mainchain |
| 10  | C8    | 1779 | GLU  | Mainchain         |
| 10  | C8    | 1780 | ARG  | Peptide,Mainchain |
| 10  | C8    | 1781 | GLY  | Mainchain         |
| 10  | C8    | 1782 | SER  | Mainchain         |
| 10  | C8    | 1783 | TYR  | Mainchain         |
| 10  | C8    | 187  | GLY  | Mainchain         |
| 10  | C8    | 248  | LEU  | Mainchain         |
| 10  | C8    | 250  | GLU  | Mainchain         |
| 10  | C8    | 251  | GLY  | Mainchain         |
| 10  | C8    | 280  | SER  | Mainchain         |
| 10  | C8    | 282  | LYS  | Mainchain         |
| 10  | C8    | 283  | SER  | Mainchain         |
| 10  | C8    | 334  | MET  | Mainchain         |
| 10  | C8    | 335  | ASP  | Peptide,Mainchain |
| 10  | C8    | 336  | THR  | Peptide,Mainchain |
| 10  | C8    | 337  | ILE  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 10  | C8    | 338  | SER  | Mainchain         |
| 10  | C8    | 423  | SER  | Mainchain         |
| 10  | C8    | 425  | PRO  | Mainchain         |
| 10  | C8    | 426  | LEU  | Mainchain         |
| 10  | C8    | 427  | ASP  | Mainchain         |
| 10  | C8    | 428  | GLY  | Peptide,Mainchain |
| 10  | C8    | 429  | SER  | Mainchain         |
| 10  | C8    | 454  | SER  | Mainchain         |
| 10  | C8    | 456  | ASN  | Mainchain         |
| 10  | C8    | 530  | THR  | Mainchain         |
| 10  | C8    | 533  | ALA  | Mainchain         |
| 10  | C8    | 620  | PRO  | Mainchain         |
| 10  | C8    | 669  | GLY  | Peptide           |
| 10  | C8    | 671  | LYS  | Peptide           |
| 10  | C8    | 672  | ASP  | Mainchain         |
| 10  | C8    | 673  | VAL  | Mainchain         |
| 10  | C8    | 674  | ASN  | Mainchain         |
| 10  | C8    | 675  | ASP  | Mainchain         |
| 10  | C8    | 677  | GLY  | Mainchain         |
| 10  | C8    | 849  | SER  | Mainchain         |
| 10  | C8    | 881  | GLU  | Mainchain         |
| 24  | D     | 1061 | SER  | Peptide           |
| 24  | D     | 1065 | ALA  | Peptide           |
| 24  | D     | 1066 | VAL  | Peptide           |
| 24  | D     | 1067 | SER  | Peptide           |
| 24  | D     | 1070 | SER  | Peptide           |
| 24  | D     | 1074 | GLY  | Peptide           |
| 24  | D     | 1151 | SER  | Peptide           |
| 24  | D     | 1199 | GLN  | Peptide           |
| 24  | D     | 1201 | GLY  | Peptide           |
| 24  | D     | 1397 | THR  | Peptide           |
| 24  | D     | 1398 | ARG  | Peptide           |
| 24  | D     | 1399 | SER  | Peptide           |
| 24  | D     | 1400 | SER  | Peptide           |
| 24  | D     | 1401 | LEU  | Peptide           |
| 24  | D     | 1403 | LEU  | Peptide           |
| 24  | D     | 1404 | GLY  | Peptide           |
| 24  | D     | 1448 | TYR  | Sidechain         |
| 24  | D     | 307  | GLY  | Peptide           |
| 24  | D     | 391  | VAL  | Peptide           |
| 24  | D     | 52   | ARG  | Sidechain         |
| 24  | D     | 634  | THR  | Peptide           |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 24  | D     | 757  | GLY  | Peptide   |
| 24  | D     | 758  | ALA  | Peptide   |
| 24  | D     | 759  | TYR  | Peptide   |
| 24  | D     | 762  | GLY  | Peptide   |
| 24  | D     | 764  | GLU  | Peptide   |
| 24  | D     | 765  | SER  | Peptide   |
| 24  | D     | 767  | ASN  | Peptide   |
| 24  | D     | 768  | LYS  | Peptide   |
| 24  | D16   | 1061 | SER  | Peptide   |
| 24  | D16   | 1065 | ALA  | Peptide   |
| 24  | D16   | 1066 | VAL  | Peptide   |
| 24  | D16   | 1067 | SER  | Peptide   |
| 24  | D16   | 1070 | SER  | Peptide   |
| 24  | D16   | 1074 | GLY  | Peptide   |
| 24  | D16   | 1151 | SER  | Peptide   |
| 24  | D16   | 1199 | GLN  | Peptide   |
| 24  | D16   | 1201 | GLY  | Peptide   |
| 24  | D16   | 1397 | THR  | Peptide   |
| 24  | D16   | 1398 | ARG  | Peptide   |
| 24  | D16   | 1399 | SER  | Peptide   |
| 24  | D16   | 1400 | SER  | Peptide   |
| 24  | D16   | 1401 | LEU  | Peptide   |
| 24  | D16   | 1403 | LEU  | Peptide   |
| 24  | D16   | 1404 | GLY  | Peptide   |
| 24  | D16   | 1448 | TYR  | Sidechain |
| 24  | D16   | 307  | GLY  | Peptide   |
| 24  | D16   | 391  | VAL  | Peptide   |
| 24  | D16   | 52   | ARG  | Sidechain |
| 24  | D16   | 634  | THR  | Peptide   |
| 24  | D16   | 757  | GLY  | Peptide   |
| 24  | D16   | 758  | ALA  | Peptide   |
| 24  | D16   | 759  | TYR  | Peptide   |
| 24  | D16   | 762  | GLY  | Peptide   |
| 24  | D16   | 764  | GLU  | Peptide   |
| 24  | D16   | 765  | SER  | Peptide   |
| 24  | D16   | 767  | ASN  | Peptide   |
| 24  | D16   | 768  | LYS  | Peptide   |
| 24  | D24   | 1061 | SER  | Peptide   |
| 24  | D24   | 1065 | ALA  | Peptide   |
| 24  | D24   | 1066 | VAL  | Peptide   |
| 24  | D24   | 1067 | SER  | Peptide   |
| 24  | D24   | 1070 | SER  | Peptide   |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 24  | D24   | 1074 | GLY  | Peptide   |
| 24  | D24   | 1151 | SER  | Peptide   |
| 24  | D24   | 1199 | GLN  | Peptide   |
| 24  | D24   | 1201 | GLY  | Peptide   |
| 24  | D24   | 1397 | THR  | Peptide   |
| 24  | D24   | 1398 | ARG  | Peptide   |
| 24  | D24   | 1399 | SER  | Peptide   |
| 24  | D24   | 1400 | SER  | Peptide   |
| 24  | D24   | 1401 | LEU  | Peptide   |
| 24  | D24   | 1403 | LEU  | Peptide   |
| 24  | D24   | 1404 | GLY  | Peptide   |
| 24  | D24   | 1448 | TYR  | Sidechain |
| 24  | D24   | 307  | GLY  | Peptide   |
| 24  | D24   | 391  | VAL  | Peptide   |
| 24  | D24   | 52   | ARG  | Sidechain |
| 24  | D24   | 634  | THR  | Peptide   |
| 24  | D24   | 757  | GLY  | Peptide   |
| 24  | D24   | 758  | ALA  | Peptide   |
| 24  | D24   | 759  | TYR  | Peptide   |
| 24  | D24   | 762  | GLY  | Peptide   |
| 24  | D24   | 764  | GLU  | Peptide   |
| 24  | D24   | 765  | SER  | Peptide   |
| 24  | D24   | 767  | ASN  | Peptide   |
| 24  | D24   | 768  | LYS  | Peptide   |
| 24  | D32   | 1061 | SER  | Peptide   |
| 24  | D32   | 1065 | ALA  | Peptide   |
| 24  | D32   | 1066 | VAL  | Peptide   |
| 24  | D32   | 1067 | SER  | Peptide   |
| 24  | D32   | 1070 | SER  | Peptide   |
| 24  | D32   | 1074 | GLY  | Peptide   |
| 24  | D32   | 1151 | SER  | Peptide   |
| 24  | D32   | 1199 | GLN  | Peptide   |
| 24  | D32   | 1201 | GLY  | Peptide   |
| 24  | D32   | 1397 | THR  | Peptide   |
| 24  | D32   | 1398 | ARG  | Peptide   |
| 24  | D32   | 1399 | SER  | Peptide   |
| 24  | D32   | 1400 | SER  | Peptide   |
| 24  | D32   | 1401 | LEU  | Peptide   |
| 24  | D32   | 1403 | LEU  | Peptide   |
| 24  | D32   | 1404 | GLY  | Peptide   |
| 24  | D32   | 1448 | TYR  | Sidechain |
| 24  | D32   | 307  | GLY  | Peptide   |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 24  | D32   | 391  | VAL  | Peptide   |
| 24  | D32   | 52   | ARG  | Sidechain |
| 24  | D32   | 634  | THR  | Peptide   |
| 24  | D32   | 757  | GLY  | Peptide   |
| 24  | D32   | 758  | ALA  | Peptide   |
| 24  | D32   | 759  | TYR  | Peptide   |
| 24  | D32   | 762  | GLY  | Peptide   |
| 24  | D32   | 764  | GLU  | Peptide   |
| 24  | D32   | 765  | SER  | Peptide   |
| 24  | D32   | 767  | ASN  | Peptide   |
| 24  | D32   | 768  | LYS  | Peptide   |
| 24  | D40   | 1061 | SER  | Peptide   |
| 24  | D40   | 1065 | ALA  | Peptide   |
| 24  | D40   | 1066 | VAL  | Peptide   |
| 24  | D40   | 1067 | SER  | Peptide   |
| 24  | D40   | 1070 | SER  | Peptide   |
| 24  | D40   | 1074 | GLY  | Peptide   |
| 24  | D40   | 1151 | SER  | Peptide   |
| 24  | D40   | 1199 | GLN  | Peptide   |
| 24  | D40   | 1201 | GLY  | Peptide   |
| 24  | D40   | 1397 | THR  | Peptide   |
| 24  | D40   | 1398 | ARG  | Peptide   |
| 24  | D40   | 1399 | SER  | Peptide   |
| 24  | D40   | 1400 | SER  | Peptide   |
| 24  | D40   | 1401 | LEU  | Peptide   |
| 24  | D40   | 1403 | LEU  | Peptide   |
| 24  | D40   | 1404 | GLY  | Peptide   |
| 24  | D40   | 1448 | TYR  | Sidechain |
| 24  | D40   | 307  | GLY  | Peptide   |
| 24  | D40   | 391  | VAL  | Peptide   |
| 24  | D40   | 52   | ARG  | Sidechain |
| 24  | D40   | 634  | THR  | Peptide   |
| 24  | D40   | 757  | GLY  | Peptide   |
| 24  | D40   | 758  | ALA  | Peptide   |
| 24  | D40   | 759  | TYR  | Peptide   |
| 24  | D40   | 762  | GLY  | Peptide   |
| 24  | D40   | 764  | GLU  | Peptide   |
| 24  | D40   | 765  | SER  | Peptide   |
| 24  | D40   | 767  | ASN  | Peptide   |
| 24  | D40   | 768  | LYS  | Peptide   |
| 24  | D8    | 1061 | SER  | Peptide   |
| 24  | D8    | 1065 | ALA  | Peptide   |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 24  | D8    | 1066 | VAL  | Peptide   |
| 24  | D8    | 1067 | SER  | Peptide   |
| 24  | D8    | 1070 | SER  | Peptide   |
| 24  | D8    | 1074 | GLY  | Peptide   |
| 24  | D8    | 1151 | SER  | Peptide   |
| 24  | D8    | 1199 | GLN  | Peptide   |
| 24  | D8    | 1201 | GLY  | Peptide   |
| 24  | D8    | 1397 | THR  | Peptide   |
| 24  | D8    | 1398 | ARG  | Peptide   |
| 24  | D8    | 1399 | SER  | Peptide   |
| 24  | D8    | 1400 | SER  | Peptide   |
| 24  | D8    | 1401 | LEU  | Peptide   |
| 24  | D8    | 1403 | LEU  | Peptide   |
| 24  | D8    | 1404 | GLY  | Peptide   |
| 24  | D8    | 1448 | TYR  | Sidechain |
| 24  | D8    | 307  | GLY  | Peptide   |
| 24  | D8    | 391  | VAL  | Peptide   |
| 24  | D8    | 52   | ARG  | Sidechain |
| 24  | D8    | 634  | THR  | Peptide   |
| 24  | D8    | 757  | GLY  | Peptide   |
| 24  | D8    | 758  | ALA  | Peptide   |
| 24  | D8    | 759  | TYR  | Peptide   |
| 24  | D8    | 762  | GLY  | Peptide   |
| 24  | D8    | 764  | GLU  | Peptide   |
| 24  | D8    | 765  | SER  | Peptide   |
| 24  | D8    | 767  | ASN  | Peptide   |
| 24  | D8    | 768  | LYS  | Peptide   |
| 20  | E     | 1    | MET  | Mainchain |
| 20  | E     | 126  | SER  | Mainchain |
| 20  | E     | 128  | SER  | Mainchain |
| 20  | E     | 2    | PRO  | Mainchain |
| 20  | E     | 200  | LEU  | Mainchain |
| 20  | E     | 201  | LEU  | Mainchain |
| 20  | E     | 202  | ASP  | Mainchain |
| 20  | E     | 203  | TRP  | Mainchain |
| 20  | E     | 204  | SER  | Mainchain |
| 20  | E     | 207  | LEU  | Mainchain |
| 20  | E     | 208  | VAL  | Mainchain |
| 20  | E     | 209  | SER  | Mainchain |
| 20  | E     | 3    | SER  | Mainchain |
| 20  | E     | 339  | LYS  | Mainchain |
| 20  | E     | 341  | TYR  | Mainchain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 20  | E     | 342 | GLN  | Mainchain         |
| 20  | E     | 344 | PRO  | Peptide,Mainchain |
| 20  | E     | 345 | LEU  | Mainchain         |
| 20  | E     | 347 | PRO  | Mainchain         |
| 20  | E     | 348 | PRO  | Mainchain         |
| 20  | E     | 349 | THR  | Mainchain         |
| 20  | E     | 350 | GLU  | Mainchain         |
| 20  | E     | 351 | SER  | Mainchain         |
| 20  | E     | 352 | PHE  | Mainchain         |
| 20  | E     | 38  | PHE  | Mainchain         |
| 20  | E     | 39  | SER  | Mainchain         |
| 20  | E     | 4   | PRO  | Mainchain         |
| 20  | E     | 417 | LYS  | Mainchain         |
| 20  | E     | 418 | THR  | Mainchain         |
| 20  | E     | 419 | ASN  | Mainchain         |
| 20  | E     | 420 | LEU  | Mainchain         |
| 20  | E     | 422 | SER  | Mainchain         |
| 20  | E     | 423 | PRO  | Mainchain         |
| 20  | E     | 424 | GLN  | Mainchain         |
| 20  | E     | 427 | MET  | Mainchain         |
| 20  | E     | 429 | PRO  | Peptide,Mainchain |
| 20  | E     | 430 | ALA  | Mainchain         |
| 20  | E     | 434 | TRP  | Mainchain         |
| 20  | E     | 435 | ALA  | Mainchain         |
| 20  | E     | 436 | THR  | Mainchain         |
| 20  | E     | 437 | SER  | Mainchain         |
| 20  | E     | 438 | SER  | Mainchain         |
| 20  | E     | 439 | MET  | Mainchain         |
| 20  | E     | 440 | VAL  | Mainchain         |
| 20  | E     | 441 | ARG  | Mainchain         |
| 20  | E     | 443 | ASP  | Mainchain         |
| 20  | E     | 444 | VAL  | Mainchain         |
| 20  | E     | 446 | PRO  | Mainchain         |
| 20  | E     | 451 | ILE  | Mainchain         |
| 20  | E8    | 1   | MET  | Mainchain         |
| 20  | E8    | 126 | SER  | Mainchain         |
| 20  | E8    | 128 | SER  | Mainchain         |
| 20  | E8    | 2   | PRO  | Mainchain         |
| 20  | E8    | 200 | LEU  | Mainchain         |
| 20  | E8    | 201 | LEU  | Mainchain         |
| 20  | E8    | 202 | ASP  | Mainchain         |
| 20  | E8    | 203 | TRP  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 20  | E8    | 204 | SER  | Mainchain         |
| 20  | E8    | 207 | LEU  | Mainchain         |
| 20  | E8    | 208 | VAL  | Mainchain         |
| 20  | E8    | 209 | SER  | Mainchain         |
| 20  | E8    | 3   | SER  | Mainchain         |
| 20  | E8    | 339 | LYS  | Mainchain         |
| 20  | E8    | 341 | TYR  | Mainchain         |
| 20  | E8    | 342 | GLN  | Mainchain         |
| 20  | E8    | 344 | PRO  | Peptide,Mainchain |
| 20  | E8    | 345 | LEU  | Mainchain         |
| 20  | E8    | 347 | PRO  | Mainchain         |
| 20  | E8    | 348 | PRO  | Mainchain         |
| 20  | E8    | 349 | THR  | Mainchain         |
| 20  | E8    | 350 | GLU  | Mainchain         |
| 20  | E8    | 351 | SER  | Mainchain         |
| 20  | E8    | 352 | PHE  | Mainchain         |
| 20  | E8    | 38  | PHE  | Mainchain         |
| 20  | E8    | 39  | SER  | Mainchain         |
| 20  | E8    | 4   | PRO  | Mainchain         |
| 20  | E8    | 417 | LYS  | Mainchain         |
| 20  | E8    | 418 | THR  | Mainchain         |
| 20  | E8    | 419 | ASN  | Mainchain         |
| 20  | E8    | 420 | LEU  | Mainchain         |
| 20  | E8    | 422 | SER  | Mainchain         |
| 20  | E8    | 423 | PRO  | Mainchain         |
| 20  | E8    | 424 | GLN  | Mainchain         |
| 20  | E8    | 427 | MET  | Mainchain         |
| 20  | E8    | 429 | PRO  | Peptide,Mainchain |
| 20  | E8    | 430 | ALA  | Mainchain         |
| 20  | E8    | 434 | TRP  | Mainchain         |
| 20  | E8    | 435 | ALA  | Mainchain         |
| 20  | E8    | 436 | THR  | Mainchain         |
| 20  | E8    | 437 | SER  | Mainchain         |
| 20  | E8    | 438 | SER  | Mainchain         |
| 20  | E8    | 439 | MET  | Mainchain         |
| 20  | E8    | 440 | VAL  | Mainchain         |
| 20  | E8    | 441 | ARG  | Mainchain         |
| 20  | E8    | 443 | ASP  | Mainchain         |
| 20  | E8    | 444 | VAL  | Mainchain         |
| 20  | E8    | 446 | PRO  | Mainchain         |
| 20  | E8    | 451 | ILE  | Mainchain         |
| 17  | F     | 68  | PHE  | Mainchain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 17  | F     | 69  | SER  | Mainchain |
| 17  | F     | 70  | PRO  | Mainchain |
| 17  | F     | 71  | GLU  | Mainchain |
| 17  | F     | 72  | SER  | Mainchain |
| 17  | F     | 73  | GLY  | Mainchain |
| 17  | F     | 74  | ILE  | Mainchain |
| 17  | F     | 77  | TYR  | Mainchain |
| 17  | F     | 78  | SER  | Mainchain |
| 17  | F     | 79  | ALA  | Mainchain |
| 17  | F16   | 68  | PHE  | Mainchain |
| 17  | F16   | 69  | SER  | Mainchain |
| 17  | F16   | 70  | PRO  | Mainchain |
| 17  | F16   | 71  | GLU  | Mainchain |
| 17  | F16   | 72  | SER  | Mainchain |
| 17  | F16   | 73  | GLY  | Mainchain |
| 17  | F16   | 74  | ILE  | Mainchain |
| 17  | F16   | 77  | TYR  | Mainchain |
| 17  | F16   | 78  | SER  | Mainchain |
| 17  | F16   | 79  | ALA  | Mainchain |
| 17  | F24   | 68  | PHE  | Mainchain |
| 17  | F24   | 69  | SER  | Mainchain |
| 17  | F24   | 70  | PRO  | Mainchain |
| 17  | F24   | 71  | GLU  | Mainchain |
| 17  | F24   | 72  | SER  | Mainchain |
| 17  | F24   | 73  | GLY  | Mainchain |
| 17  | F24   | 74  | ILE  | Mainchain |
| 17  | F24   | 77  | TYR  | Mainchain |
| 17  | F24   | 78  | SER  | Mainchain |
| 17  | F24   | 79  | ALA  | Mainchain |
| 17  | F8    | 68  | PHE  | Mainchain |
| 17  | F8    | 69  | SER  | Mainchain |
| 17  | F8    | 70  | PRO  | Mainchain |
| 17  | F8    | 71  | GLU  | Mainchain |
| 17  | F8    | 72  | SER  | Mainchain |
| 17  | F8    | 73  | GLY  | Mainchain |
| 17  | F8    | 74  | ILE  | Mainchain |
| 17  | F8    | 77  | TYR  | Mainchain |
| 17  | F8    | 78  | SER  | Mainchain |
| 17  | F8    | 79  | ALA  | Mainchain |
| 21  | H     | 138 | GLU  | Mainchain |
| 21  | H     | 318 | ALA  | Mainchain |
| 21  | H     | 319 | GLY  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 21  | H     | 320 | SER  | Mainchain |
| 21  | H     | 321 | SER  | Mainchain |
| 21  | H     | 322 | LEU  | Mainchain |
| 21  | H     | 323 | TYR  | Mainchain |
| 21  | H     | 326 | GLY  | Mainchain |
| 21  | H16   | 138 | GLU  | Mainchain |
| 21  | H16   | 318 | ALA  | Mainchain |
| 21  | H16   | 319 | GLY  | Mainchain |
| 21  | H16   | 320 | SER  | Mainchain |
| 21  | H16   | 321 | SER  | Mainchain |
| 21  | H16   | 322 | LEU  | Mainchain |
| 21  | H16   | 323 | TYR  | Mainchain |
| 21  | H16   | 326 | GLY  | Mainchain |
| 21  | H24   | 138 | GLU  | Mainchain |
| 21  | H24   | 318 | ALA  | Mainchain |
| 21  | H24   | 319 | GLY  | Mainchain |
| 21  | H24   | 320 | SER  | Mainchain |
| 21  | H24   | 321 | SER  | Mainchain |
| 21  | H24   | 322 | LEU  | Mainchain |
| 21  | H24   | 323 | TYR  | Mainchain |
| 21  | H24   | 326 | GLY  | Mainchain |
| 21  | H8    | 138 | GLU  | Mainchain |
| 21  | H8    | 318 | ALA  | Mainchain |
| 21  | H8    | 319 | GLY  | Mainchain |
| 21  | H8    | 320 | SER  | Mainchain |
| 21  | H8    | 321 | SER  | Mainchain |
| 21  | H8    | 322 | LEU  | Mainchain |
| 21  | H8    | 323 | TYR  | Mainchain |
| 21  | H8    | 326 | GLY  | Mainchain |
| 22  | I     | 149 | SER  | Mainchain |
| 22  | I     | 206 | PHE  | Mainchain |
| 22  | I     | 207 | PRO  | Mainchain |
| 22  | I     | 209 | TRP  | Mainchain |
| 22  | I     | 252 | ARG  | Mainchain |
| 22  | I     | 296 | ARG  | Mainchain |
| 22  | I     | 297 | HIS  | Mainchain |
| 22  | I     | 298 | ALA  | Mainchain |
| 22  | I     | 299 | SER  | Mainchain |
| 22  | I     | 369 | HIS  | Mainchain |
| 22  | I     | 370 | PRO  | Mainchain |
| 22  | I     | 371 | THR  | Mainchain |
| 22  | I16   | 149 | SER  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 22  | I16   | 206 | PHE  | Mainchain |
| 22  | I16   | 207 | PRO  | Mainchain |
| 22  | I16   | 209 | TRP  | Mainchain |
| 22  | I16   | 252 | ARG  | Mainchain |
| 22  | I16   | 296 | ARG  | Mainchain |
| 22  | I16   | 297 | HIS  | Mainchain |
| 22  | I16   | 298 | ALA  | Mainchain |
| 22  | I16   | 299 | SER  | Mainchain |
| 22  | I16   | 369 | HIS  | Mainchain |
| 22  | I16   | 370 | PRO  | Mainchain |
| 22  | I16   | 371 | THR  | Mainchain |
| 22  | I24   | 149 | SER  | Mainchain |
| 22  | I24   | 206 | PHE  | Mainchain |
| 22  | I24   | 207 | PRO  | Mainchain |
| 22  | I24   | 209 | TRP  | Mainchain |
| 22  | I24   | 252 | ARG  | Mainchain |
| 22  | I24   | 296 | ARG  | Mainchain |
| 22  | I24   | 297 | HIS  | Mainchain |
| 22  | I24   | 298 | ALA  | Mainchain |
| 22  | I24   | 299 | SER  | Mainchain |
| 22  | I24   | 369 | HIS  | Mainchain |
| 22  | I24   | 370 | PRO  | Mainchain |
| 22  | I24   | 371 | THR  | Mainchain |
| 22  | I8    | 149 | SER  | Mainchain |
| 22  | I8    | 206 | PHE  | Mainchain |
| 22  | I8    | 207 | PRO  | Mainchain |
| 22  | I8    | 209 | TRP  | Mainchain |
| 22  | I8    | 252 | ARG  | Mainchain |
| 22  | I8    | 296 | ARG  | Mainchain |
| 22  | I8    | 297 | HIS  | Mainchain |
| 22  | I8    | 298 | ALA  | Mainchain |
| 22  | I8    | 299 | SER  | Mainchain |
| 22  | I8    | 369 | HIS  | Mainchain |
| 22  | I8    | 370 | PRO  | Mainchain |
| 22  | I8    | 371 | THR  | Mainchain |
| 15  | J     | 542 | THR  | Mainchain |
| 15  | J     | 677 | GLY  | Mainchain |
| 15  | J     | 679 | GLU  | Mainchain |
| 15  | J     | 680 | LEU  | Mainchain |
| 15  | J     | 682 | ALA  | Mainchain |
| 15  | J     | 684 | ASP  | Mainchain |
| 15  | J     | 687 | SER  | Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 23  | J16   | 679  | GLU  | Mainchain         |
| 23  | J16   | 681  | GLU  | Mainchain         |
| 23  | J16   | 682  | ALA  | Mainchain         |
| 23  | J16   | 683  | ILE  | Mainchain         |
| 23  | J16   | 684  | ASP  | Mainchain         |
| 23  | J16   | 724  | GLY  | Mainchain         |
| 23  | J16   | 726  | GLY  | Mainchain         |
| 23  | J16   | 733  | ALA  | Mainchain         |
| 23  | J16   | 735  | LYS  | Mainchain         |
| 23  | J24   | 679  | GLU  | Mainchain         |
| 23  | J24   | 681  | GLU  | Mainchain         |
| 23  | J24   | 682  | ALA  | Mainchain         |
| 23  | J24   | 683  | ILE  | Mainchain         |
| 23  | J24   | 684  | ASP  | Mainchain         |
| 23  | J24   | 724  | GLY  | Mainchain         |
| 23  | J24   | 726  | GLY  | Mainchain         |
| 23  | J24   | 733  | ALA  | Mainchain         |
| 23  | J24   | 735  | LYS  | Mainchain         |
| 23  | J32   | 679  | GLU  | Mainchain         |
| 23  | J32   | 681  | GLU  | Mainchain         |
| 23  | J32   | 682  | ALA  | Mainchain         |
| 23  | J32   | 683  | ILE  | Mainchain         |
| 23  | J32   | 684  | ASP  | Mainchain         |
| 23  | J32   | 724  | GLY  | Mainchain         |
| 23  | J32   | 726  | GLY  | Mainchain         |
| 23  | J32   | 733  | ALA  | Mainchain         |
| 23  | J32   | 735  | LYS  | Mainchain         |
| 23  | J8    | 679  | GLU  | Mainchain         |
| 23  | J8    | 681  | GLU  | Mainchain         |
| 23  | J8    | 682  | ALA  | Mainchain         |
| 23  | J8    | 683  | ILE  | Mainchain         |
| 23  | J8    | 684  | ASP  | Mainchain         |
| 23  | J8    | 724  | GLY  | Mainchain         |
| 23  | J8    | 726  | GLY  | Mainchain         |
| 23  | J8    | 733  | ALA  | Mainchain         |
| 23  | J8    | 735  | LYS  | Mainchain         |
| 9   | K     | 1047 | SER  | Mainchain         |
| 9   | K     | 1048 | GLN  | Mainchain         |
| 9   | K     | 1049 | ASP  | Peptide,Mainchain |
| 9   | K     | 1051 | GLU  | Mainchain         |
| 9   | K     | 1052 | SER  | Mainchain         |
| 9   | K     | 1053 | MET  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 9   | K     | 1054 | THR  | Peptide,Mainchain |
| 9   | K     | 1056 | VAL  | Mainchain         |
| 9   | K     | 1057 | GLU  | Peptide,Mainchain |
| 9   | K     | 1058 | GLU  | Mainchain         |
| 9   | K     | 1059 | ARG  | Mainchain         |
| 9   | K     | 1060 | THR  | Mainchain         |
| 9   | K     | 1062 | PRO  | Mainchain         |
| 9   | K     | 1063 | GLU  | Mainchain         |
| 9   | K     | 1064 | PRO  | Mainchain         |
| 9   | K     | 1065 | GLU  | Mainchain         |
| 9   | K     | 1066 | ASP  | Mainchain         |
| 9   | K     | 1067 | VAL  | Mainchain         |
| 9   | K     | 1068 | GLN  | Mainchain         |
| 9   | K     | 1069 | PRO  | Mainchain         |
| 9   | K     | 1088 | ASP  | Mainchain         |
| 9   | K     | 1089 | LYS  | Mainchain         |
| 9   | K     | 1091 | ALA  | Mainchain         |
| 9   | K     | 1117 | LEU  | Mainchain         |
| 9   | K     | 1119 | ASN  | Mainchain         |
| 9   | K     | 1120 | GLY  | Mainchain         |
| 9   | K     | 1126 | LEU  | Mainchain         |
| 9   | K     | 1139 | ILE  | Mainchain         |
| 9   | K     | 1190 | GLU  | Mainchain         |
| 9   | K     | 1218 | ARG  | Mainchain         |
| 9   | K     | 1220 | ASN  | Mainchain         |
| 9   | K     | 1222 | PHE  | Mainchain         |
| 9   | K     | 1234 | ARG  | Mainchain         |
| 9   | K     | 1235 | GLU  | Mainchain         |
| 9   | K     | 1237 | PRO  | Mainchain         |
| 9   | K     | 1238 | GLU  | Mainchain         |
| 9   | K     | 1239 | ASP  | Mainchain         |
| 9   | K     | 1241 | THR  | Mainchain         |
| 9   | K     | 1242 | SER  | Mainchain         |
| 9   | K     | 1271 | GLU  | Mainchain         |
| 9   | K     | 1273 | GLU  | Mainchain         |
| 9   | K     | 1274 | GLY  | Mainchain         |
| 9   | K     | 1277 | ALA  | Mainchain         |
| 9   | K     | 1278 | GLU  | Peptide,Mainchain |
| 9   | K     | 1279 | GLU  | Mainchain         |
| 9   | K     | 1280 | PHE  | Mainchain         |
| 9   | K     | 1281 | SER  | Mainchain         |
| 9   | K     | 1282 | SER  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 9   | K     | 577  | GLN  | Mainchain         |
| 9   | K     | 638  | TRP  | Mainchain         |
| 9   | K     | 639  | THR  | Mainchain         |
| 9   | K     | 640  | THR  | Mainchain         |
| 9   | K     | 641  | THR  | Mainchain         |
| 9   | K     | 643  | GLY  | Mainchain         |
| 9   | K     | 644  | ALA  | Mainchain         |
| 9   | K     | 718  | PHE  | Mainchain         |
| 9   | K     | 721  | PRO  | Mainchain         |
| 9   | K     | 722  | GLN  | Peptide,Mainchain |
| 9   | K     | 725  | SER  | Peptide,Mainchain |
| 9   | K     | 726  | GLU  | Mainchain         |
| 9   | K     | 727  | ASP  | Mainchain         |
| 9   | K     | 728  | GLN  | Mainchain         |
| 9   | K     | 729  | VAL  | Mainchain         |
| 9   | K     | 730  | SER  | Mainchain         |
| 9   | K     | 731  | CYS  | Mainchain         |
| 9   | K     | 857  | ASP  | Mainchain         |
| 9   | K     | 889  | ARG  | Mainchain         |
| 9   | K     | 890  | GLU  | Mainchain         |
| 9   | K     | 891  | GLU  | Mainchain         |
| 9   | K     | 893  | ASN  | Mainchain         |
| 9   | K     | 926  | ILE  | Mainchain         |
| 9   | K     | 927  | ARG  | Mainchain         |
| 9   | K     | 928  | GLU  | Mainchain         |
| 9   | K     | 929  | ARG  | Mainchain         |
| 9   | K     | 930  | THR  | Mainchain         |
| 9   | K     | 965  | LEU  | Mainchain         |
| 9   | K     | 978  | GLY  | Mainchain         |
| 9   | K16   | 1054 | THR  | Peptide           |
| 9   | K16   | 1058 | GLU  | Peptide           |
| 9   | K16   | 1212 | ARG  | Sidechain         |
| 9   | K16   | 643  | GLY  | Peptide           |
| 9   | K16   | 723  | ALA  | Peptide           |
| 9   | K16   | 724  | GLY  | Peptide           |
| 9   | K8    | 1047 | SER  | Mainchain         |
| 9   | K8    | 1048 | GLN  | Mainchain         |
| 9   | K8    | 1049 | ASP  | Peptide,Mainchain |
| 9   | K8    | 1051 | GLU  | Mainchain         |
| 9   | K8    | 1052 | SER  | Mainchain         |
| 9   | K8    | 1053 | MET  | Peptide,Mainchain |
| 9   | K8    | 1054 | THR  | Peptide,Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 9   | K8    | 1056 | VAL  | Mainchain         |
| 9   | K8    | 1057 | GLU  | Peptide,Mainchain |
| 9   | K8    | 1058 | GLU  | Mainchain         |
| 9   | K8    | 1059 | ARG  | Mainchain         |
| 9   | K8    | 1060 | THR  | Mainchain         |
| 9   | K8    | 1062 | PRO  | Mainchain         |
| 9   | K8    | 1063 | GLU  | Mainchain         |
| 9   | K8    | 1064 | PRO  | Mainchain         |
| 9   | K8    | 1065 | GLU  | Mainchain         |
| 9   | K8    | 1066 | ASP  | Mainchain         |
| 9   | K8    | 1067 | VAL  | Mainchain         |
| 9   | K8    | 1068 | GLN  | Mainchain         |
| 9   | K8    | 1069 | PRO  | Mainchain         |
| 9   | K8    | 1088 | ASP  | Mainchain         |
| 9   | K8    | 1089 | LYS  | Mainchain         |
| 9   | K8    | 1091 | ALA  | Mainchain         |
| 9   | K8    | 1117 | LEU  | Mainchain         |
| 9   | K8    | 1119 | ASN  | Mainchain         |
| 9   | K8    | 1120 | GLY  | Mainchain         |
| 9   | K8    | 1126 | LEU  | Mainchain         |
| 9   | K8    | 1139 | ILE  | Mainchain         |
| 9   | K8    | 1190 | GLU  | Mainchain         |
| 9   | K8    | 1218 | ARG  | Mainchain         |
| 9   | K8    | 1220 | ASN  | Mainchain         |
| 9   | K8    | 1222 | PHE  | Mainchain         |
| 9   | K8    | 1234 | ARG  | Mainchain         |
| 9   | K8    | 1235 | GLU  | Mainchain         |
| 9   | K8    | 1237 | PRO  | Mainchain         |
| 9   | K8    | 1238 | GLU  | Mainchain         |
| 9   | K8    | 1239 | ASP  | Mainchain         |
| 9   | K8    | 1241 | THR  | Mainchain         |
| 9   | K8    | 1242 | SER  | Mainchain         |
| 9   | K8    | 1271 | GLU  | Mainchain         |
| 9   | K8    | 1273 | GLU  | Mainchain         |
| 9   | K8    | 1274 | GLY  | Mainchain         |
| 9   | K8    | 1277 | ALA  | Mainchain         |
| 9   | K8    | 1278 | GLU  | Peptide,Mainchain |
| 9   | K8    | 1279 | GLU  | Mainchain         |
| 9   | K8    | 1280 | PHE  | Mainchain         |
| 9   | K8    | 1281 | SER  | Mainchain         |
| 9   | K8    | 1282 | SER  | Mainchain         |
| 9   | K8    | 577  | GLN  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 9   | K8    | 638  | TRP  | Mainchain         |
| 9   | K8    | 639  | THR  | Mainchain         |
| 9   | K8    | 640  | THR  | Mainchain         |
| 9   | K8    | 641  | THR  | Mainchain         |
| 9   | K8    | 643  | GLY  | Mainchain         |
| 9   | K8    | 644  | ALA  | Mainchain         |
| 9   | K8    | 718  | PHE  | Mainchain         |
| 9   | K8    | 721  | PRO  | Mainchain         |
| 9   | K8    | 722  | GLN  | Peptide,Mainchain |
| 9   | K8    | 725  | SER  | Peptide,Mainchain |
| 9   | K8    | 726  | GLU  | Mainchain         |
| 9   | K8    | 727  | ASP  | Mainchain         |
| 9   | K8    | 728  | GLN  | Mainchain         |
| 9   | K8    | 729  | VAL  | Mainchain         |
| 9   | K8    | 730  | SER  | Mainchain         |
| 9   | K8    | 731  | CYS  | Mainchain         |
| 9   | K8    | 857  | ASP  | Mainchain         |
| 9   | K8    | 889  | ARG  | Mainchain         |
| 9   | K8    | 890  | GLU  | Mainchain         |
| 9   | K8    | 891  | GLU  | Mainchain         |
| 9   | K8    | 893  | ASN  | Mainchain         |
| 9   | K8    | 926  | ILE  | Mainchain         |
| 9   | K8    | 927  | ARG  | Mainchain         |
| 9   | K8    | 928  | GLU  | Mainchain         |
| 9   | K8    | 929  | ARG  | Mainchain         |
| 9   | K8    | 930  | THR  | Mainchain         |
| 9   | K8    | 965  | LEU  | Mainchain         |
| 9   | K8    | 978  | GLY  | Mainchain         |
| 8   | L     | 1085 | ARG  | Sidechain         |
| 8   | L     | 269  | TYR  | Sidechain         |
| 8   | L     | 477  | GLY  | Peptide           |
| 8   | L16   | 1085 | ARG  | Sidechain         |
| 8   | L16   | 269  | TYR  | Sidechain         |
| 8   | L16   | 477  | GLY  | Peptide           |
| 8   | L8    | 1085 | ARG  | Sidechain         |
| 8   | L8    | 269  | TYR  | Sidechain         |
| 8   | L8    | 477  | GLY  | Peptide           |
| 2   | M     | 156  | GLY  | Mainchain         |
| 2   | M     | 206  | SER  | Mainchain         |
| 2   | M     | 208  | SER  | Mainchain         |
| 2   | M     | 326  | GLN  | Mainchain         |
| 2   | M     | 327  | SER  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | M     | 332 | MET  | Mainchain         |
| 2   | M     | 336 | SER  | Mainchain         |
| 2   | M     | 337 | ASP  | Mainchain         |
| 2   | M     | 338 | ASN  | Mainchain         |
| 2   | M     | 339 | GLU  | Peptide,Mainchain |
| 2   | M     | 340 | GLU  | Mainchain         |
| 2   | M     | 341 | ASP  | Mainchain         |
| 2   | M     | 342 | VAL  | Mainchain         |
| 2   | M     | 343 | MET  | Mainchain         |
| 2   | M     | 344 | GLN  | Mainchain         |
| 2   | M     | 345 | ASP  | Mainchain         |
| 2   | M     | 346 | VAL  | Mainchain         |
| 2   | M     | 347 | LYS  | Mainchain         |
| 2   | M     | 348 | GLU  | Mainchain         |
| 2   | M     | 349 | ASP  | Mainchain         |
| 2   | M     | 350 | SER  | Mainchain         |
| 2   | M     | 351 | ALA  | Mainchain         |
| 2   | M     | 352 | LYS  | Mainchain         |
| 2   | M     | 353 | ILE  | Mainchain         |
| 2   | M     | 386 | ASN  | Mainchain         |
| 2   | M     | 389 | SER  | Mainchain         |
| 2   | M     | 526 | ASP  | Mainchain         |
| 2   | M     | 755 | THR  | Mainchain         |
| 2   | M     | 756 | MET  | Mainchain         |
| 2   | M     | 758 | GLU  | Mainchain         |
| 2   | M     | 759 | LEU  | Mainchain         |
| 2   | M     | 761 | PRO  | Mainchain         |
| 2   | M16   | 156 | GLY  | Mainchain         |
| 2   | M16   | 206 | SER  | Mainchain         |
| 2   | M16   | 208 | SER  | Mainchain         |
| 2   | M16   | 326 | GLN  | Mainchain         |
| 2   | M16   | 327 | SER  | Mainchain         |
| 2   | M16   | 332 | MET  | Mainchain         |
| 2   | M16   | 336 | SER  | Mainchain         |
| 2   | M16   | 337 | ASP  | Mainchain         |
| 2   | M16   | 338 | ASN  | Mainchain         |
| 2   | M16   | 339 | GLU  | Peptide,Mainchain |
| 2   | M16   | 340 | GLU  | Mainchain         |
| 2   | M16   | 341 | ASP  | Mainchain         |
| 2   | M16   | 342 | VAL  | Mainchain         |
| 2   | M16   | 343 | MET  | Mainchain         |
| 2   | M16   | 344 | GLN  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | M16   | 345 | ASP  | Mainchain         |
| 2   | M16   | 346 | VAL  | Mainchain         |
| 2   | M16   | 347 | LYS  | Mainchain         |
| 2   | M16   | 348 | GLU  | Mainchain         |
| 2   | M16   | 349 | ASP  | Mainchain         |
| 2   | M16   | 350 | SER  | Mainchain         |
| 2   | M16   | 351 | ALA  | Mainchain         |
| 2   | M16   | 352 | LYS  | Mainchain         |
| 2   | M16   | 353 | ILE  | Mainchain         |
| 2   | M16   | 354 | ASP  | Mainchain         |
| 2   | M16   | 386 | ASN  | Mainchain         |
| 2   | M16   | 389 | SER  | Mainchain         |
| 2   | M16   | 526 | ASP  | Mainchain         |
| 2   | M16   | 755 | THR  | Mainchain         |
| 2   | M16   | 756 | MET  | Mainchain         |
| 2   | M16   | 758 | GLU  | Mainchain         |
| 2   | M16   | 759 | LEU  | Mainchain         |
| 2   | M16   | 761 | PRO  | Mainchain         |
| 2   | M8    | 156 | GLY  | Mainchain         |
| 2   | M8    | 206 | SER  | Mainchain         |
| 2   | M8    | 208 | SER  | Mainchain         |
| 2   | M8    | 326 | GLN  | Mainchain         |
| 2   | M8    | 327 | SER  | Mainchain         |
| 2   | M8    | 332 | MET  | Mainchain         |
| 2   | M8    | 336 | SER  | Mainchain         |
| 2   | M8    | 337 | ASP  | Mainchain         |
| 2   | M8    | 338 | ASN  | Mainchain         |
| 2   | M8    | 339 | GLU  | Peptide,Mainchain |
| 2   | M8    | 340 | GLU  | Mainchain         |
| 2   | M8    | 341 | ASP  | Mainchain         |
| 2   | M8    | 342 | VAL  | Mainchain         |
| 2   | M8    | 343 | MET  | Mainchain         |
| 2   | M8    | 344 | GLN  | Mainchain         |
| 2   | M8    | 345 | ASP  | Mainchain         |
| 2   | M8    | 346 | VAL  | Mainchain         |
| 2   | M8    | 347 | LYS  | Mainchain         |
| 2   | M8    | 348 | GLU  | Mainchain         |
| 2   | M8    | 349 | ASP  | Mainchain         |
| 2   | M8    | 350 | SER  | Mainchain         |
| 2   | M8    | 351 | ALA  | Mainchain         |
| 2   | M8    | 352 | LYS  | Mainchain         |
| 2   | M8    | 353 | ILE  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | M8    | 386 | ASN  | Mainchain         |
| 2   | M8    | 389 | SER  | Mainchain         |
| 2   | M8    | 526 | ASP  | Mainchain         |
| 2   | M8    | 755 | THR  | Mainchain         |
| 2   | M8    | 756 | MET  | Mainchain         |
| 2   | M8    | 758 | GLU  | Mainchain         |
| 2   | M8    | 759 | LEU  | Mainchain         |
| 2   | M8    | 761 | PRO  | Mainchain         |
| 3   | N     | 1   | MET  | Mainchain         |
| 3   | N     | 164 | PRO  | Mainchain         |
| 3   | N     | 166 | ALA  | Mainchain         |
| 3   | N     | 167 | LEU  | Mainchain         |
| 3   | N     | 168 | VAL  | Mainchain         |
| 3   | N     | 169 | SER  | Mainchain         |
| 3   | N     | 170 | SER  | Mainchain         |
| 3   | N     | 171 | GLY  | Peptide,Mainchain |
| 3   | N     | 2   | PRO  | Mainchain         |
| 3   | N     | 220 | PRO  | Mainchain         |
| 3   | N     | 259 | MET  | Mainchain         |
| 3   | N     | 3   | GLY  | Mainchain         |
| 3   | N     | 45  | GLY  | Mainchain         |
| 3   | N16   | 1   | MET  | Mainchain         |
| 3   | N16   | 164 | PRO  | Mainchain         |
| 3   | N16   | 166 | ALA  | Mainchain         |
| 3   | N16   | 167 | LEU  | Mainchain         |
| 3   | N16   | 168 | VAL  | Mainchain         |
| 3   | N16   | 169 | SER  | Mainchain         |
| 3   | N16   | 170 | SER  | Mainchain         |
| 3   | N16   | 171 | GLY  | Peptide,Mainchain |
| 3   | N16   | 2   | PRO  | Mainchain         |
| 3   | N16   | 220 | PRO  | Mainchain         |
| 3   | N16   | 259 | MET  | Mainchain         |
| 3   | N16   | 3   | GLY  | Mainchain         |
| 3   | N16   | 45  | GLY  | Mainchain         |
| 3   | N8    | 1   | MET  | Mainchain         |
| 3   | N8    | 164 | PRO  | Mainchain         |
| 3   | N8    | 166 | ALA  | Mainchain         |
| 3   | N8    | 167 | LEU  | Mainchain         |
| 3   | N8    | 168 | VAL  | Mainchain         |
| 3   | N8    | 169 | SER  | Mainchain         |
| 3   | N8    | 170 | SER  | Mainchain         |
| 3   | N8    | 171 | GLY  | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | N8    | 2   | PRO  | Mainchain |
| 3   | N8    | 220 | PRO  | Mainchain |
| 3   | N8    | 259 | MET  | Mainchain |
| 3   | N8    | 3   | GLY  | Mainchain |
| 3   | N8    | 45  | GLY  | Mainchain |
| 6   | O     | 158 | ASP  | Mainchain |
| 6   | O     | 161 | SER  | Mainchain |
| 6   | O     | 162 | THR  | Mainchain |
| 6   | O     | 163 | LEU  | Mainchain |
| 6   | O     | 178 | MET  | Mainchain |
| 6   | O     | 179 | LYS  | Mainchain |
| 6   | O     | 180 | GLY  | Mainchain |
| 6   | O     | 277 | SER  | Mainchain |
| 6   | O     | 93  | HIS  | Mainchain |
| 6   | O16   | 158 | ASP  | Mainchain |
| 6   | O16   | 161 | SER  | Mainchain |
| 6   | O16   | 162 | THR  | Mainchain |
| 6   | O16   | 163 | LEU  | Mainchain |
| 6   | O16   | 178 | MET  | Mainchain |
| 6   | O16   | 179 | LYS  | Mainchain |
| 6   | O16   | 180 | GLY  | Mainchain |
| 6   | O16   | 277 | SER  | Mainchain |
| 6   | O16   | 93  | HIS  | Mainchain |
| 6   | O8    | 158 | ASP  | Mainchain |
| 6   | O8    | 161 | SER  | Mainchain |
| 6   | O8    | 162 | THR  | Mainchain |
| 6   | O8    | 163 | LEU  | Mainchain |
| 6   | O8    | 178 | MET  | Mainchain |
| 6   | O8    | 179 | LYS  | Mainchain |
| 6   | O8    | 180 | GLY  | Mainchain |
| 6   | O8    | 277 | SER  | Mainchain |
| 6   | O8    | 93  | HIS  | Mainchain |
| 5   | P     | 1   | MET  | Mainchain |
| 5   | P     | 10  | GLY  | Mainchain |
| 5   | P     | 11  | GLY  | Mainchain |
| 5   | P     | 12  | GLU  | Mainchain |
| 5   | P     | 13  | LEU  | Mainchain |
| 5   | P     | 142 | SER  | Mainchain |
| 5   | P     | 143 | ASN  | Mainchain |
| 5   | P     | 145 | ILE  | Mainchain |
| 5   | P     | 146 | SER  | Mainchain |
| 5   | P     | 147 | LEU  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | P     | 148 | PRO  | Mainchain |
| 5   | P     | 16  | PHE  | Mainchain |
| 5   | P     | 161 | ASN  | Mainchain |
| 5   | P     | 17  | SER  | Mainchain |
| 5   | P     | 19  | LYS  | Mainchain |
| 5   | P     | 2   | PRO  | Mainchain |
| 5   | P     | 20  | GLU  | Mainchain |
| 5   | P     | 21  | LYS  | Mainchain |
| 5   | P     | 3   | GLY  | Mainchain |
| 5   | P     | 392 | PRO  | Mainchain |
| 5   | P     | 394 | ASN  | Mainchain |
| 5   | P     | 4   | MET  | Mainchain |
| 5   | P     | 5   | SER  | Mainchain |
| 5   | P     | 59  | LEU  | Mainchain |
| 5   | P     | 592 | SER  | Mainchain |
| 5   | P     | 595 | SER  | Mainchain |
| 5   | P     | 596 | GLY  | Mainchain |
| 5   | P     | 6   | SER  | Mainchain |
| 5   | P     | 685 | PRO  | Mainchain |
| 5   | P     | 7   | GLU  | Mainchain |
| 5   | P     | 76  | LEU  | Mainchain |
| 5   | P     | 8   | SER  | Mainchain |
| 5   | P     | 9   | GLY  | Mainchain |
| 5   | P16   | 1   | MET  | Mainchain |
| 5   | P16   | 10  | GLY  | Mainchain |
| 5   | P16   | 11  | GLY  | Mainchain |
| 5   | P16   | 12  | GLU  | Mainchain |
| 5   | P16   | 13  | LEU  | Mainchain |
| 5   | P16   | 142 | SER  | Mainchain |
| 5   | P16   | 143 | ASN  | Mainchain |
| 5   | P16   | 145 | ILE  | Mainchain |
| 5   | P16   | 146 | SER  | Mainchain |
| 5   | P16   | 147 | LEU  | Mainchain |
| 5   | P16   | 148 | PRO  | Mainchain |
| 5   | P16   | 16  | PHE  | Mainchain |
| 5   | P16   | 161 | ASN  | Mainchain |
| 5   | P16   | 17  | SER  | Mainchain |
| 5   | P16   | 19  | LYS  | Mainchain |
| 5   | P16   | 2   | PRO  | Mainchain |
| 5   | P16   | 20  | GLU  | Mainchain |
| 5   | P16   | 21  | LYS  | Mainchain |
| 5   | P16   | 3   | GLY  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | P16   | 392 | PRO  | Mainchain |
| 5   | P16   | 394 | ASN  | Mainchain |
| 5   | P16   | 4   | MET  | Mainchain |
| 5   | P16   | 5   | SER  | Mainchain |
| 5   | P16   | 59  | LEU  | Mainchain |
| 5   | P16   | 592 | SER  | Mainchain |
| 5   | P16   | 595 | SER  | Mainchain |
| 5   | P16   | 596 | GLY  | Mainchain |
| 5   | P16   | 6   | SER  | Mainchain |
| 5   | P16   | 685 | PRO  | Mainchain |
| 5   | P16   | 7   | GLU  | Mainchain |
| 5   | P16   | 76  | LEU  | Mainchain |
| 5   | P16   | 8   | SER  | Mainchain |
| 5   | P16   | 9   | GLY  | Mainchain |
| 5   | P8    | 1   | MET  | Mainchain |
| 5   | P8    | 10  | GLY  | Mainchain |
| 5   | P8    | 11  | GLY  | Mainchain |
| 5   | P8    | 12  | GLU  | Mainchain |
| 5   | P8    | 13  | LEU  | Mainchain |
| 5   | P8    | 142 | SER  | Mainchain |
| 5   | P8    | 143 | ASN  | Mainchain |
| 5   | P8    | 145 | ILE  | Mainchain |
| 5   | P8    | 146 | SER  | Mainchain |
| 5   | P8    | 147 | LEU  | Mainchain |
| 5   | P8    | 148 | PRO  | Mainchain |
| 5   | P8    | 16  | PHE  | Mainchain |
| 5   | P8    | 161 | ASN  | Mainchain |
| 5   | P8    | 17  | SER  | Mainchain |
| 5   | P8    | 19  | LYS  | Mainchain |
| 5   | P8    | 2   | PRO  | Mainchain |
| 5   | P8    | 20  | GLU  | Mainchain |
| 5   | P8    | 21  | LYS  | Mainchain |
| 5   | P8    | 3   | GLY  | Mainchain |
| 5   | P8    | 392 | PRO  | Mainchain |
| 5   | P8    | 394 | ASN  | Mainchain |
| 5   | P8    | 4   | MET  | Mainchain |
| 5   | P8    | 5   | SER  | Mainchain |
| 5   | P8    | 59  | LEU  | Mainchain |
| 5   | P8    | 592 | SER  | Mainchain |
| 5   | P8    | 595 | SER  | Mainchain |
| 5   | P8    | 596 | GLY  | Mainchain |
| 5   | P8    | 6   | SER  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | P8    | 685 | PRO  | Mainchain |
| 5   | P8    | 7   | GLU  | Mainchain |
| 5   | P8    | 76  | LEU  | Mainchain |
| 5   | P8    | 8   | SER  | Mainchain |
| 5   | P8    | 9   | GLY  | Mainchain |
| 7   | Q     | 144 | GLU  | Mainchain |
| 7   | Q     | 218 | LYS  | Mainchain |
| 7   | Q     | 222 | PHE  | Mainchain |
| 7   | Q     | 271 | ALA  | Mainchain |
| 7   | Q     | 272 | SER  | Mainchain |
| 7   | Q     | 275 | ILE  | Mainchain |
| 7   | Q     | 276 | ASN  | Mainchain |
| 7   | Q     | 294 | LYS  | Mainchain |
| 7   | Q     | 295 | SER  | Mainchain |
| 7   | Q     | 297 | VAL  | Mainchain |
| 7   | Q     | 298 | SER  | Mainchain |
| 7   | Q     | 300 | SER  | Mainchain |
| 7   | Q     | 88  | ASN  | Mainchain |
| 7   | Q     | 89  | GLY  | Mainchain |
| 7   | Q     | 90  | GLY  | Mainchain |
| 7   | Q     | 92  | GLY  | Mainchain |
| 7   | Q     | 94  | SER  | Mainchain |
| 7   | Q16   | 144 | GLU  | Mainchain |
| 7   | Q16   | 218 | LYS  | Mainchain |
| 7   | Q16   | 222 | PHE  | Mainchain |
| 7   | Q16   | 271 | ALA  | Mainchain |
| 7   | Q16   | 272 | SER  | Mainchain |
| 7   | Q16   | 275 | ILE  | Mainchain |
| 7   | Q16   | 276 | ASN  | Mainchain |
| 7   | Q16   | 294 | LYS  | Mainchain |
| 7   | Q16   | 295 | SER  | Mainchain |
| 7   | Q16   | 297 | VAL  | Mainchain |
| 7   | Q16   | 298 | SER  | Mainchain |
| 7   | Q16   | 300 | SER  | Mainchain |
| 7   | Q16   | 88  | ASN  | Mainchain |
| 7   | Q16   | 89  | GLY  | Mainchain |
| 7   | Q16   | 90  | GLY  | Mainchain |
| 7   | Q16   | 92  | GLY  | Mainchain |
| 7   | Q16   | 94  | SER  | Mainchain |
| 7   | Q8    | 144 | GLU  | Mainchain |
| 7   | Q8    | 218 | LYS  | Mainchain |
| 7   | Q8    | 222 | PHE  | Mainchain |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 7   | Q8    | 271  | ALA  | Mainchain         |
| 7   | Q8    | 272  | SER  | Mainchain         |
| 7   | Q8    | 275  | ILE  | Mainchain         |
| 7   | Q8    | 276  | ASN  | Mainchain         |
| 7   | Q8    | 294  | LYS  | Mainchain         |
| 7   | Q8    | 295  | SER  | Mainchain         |
| 7   | Q8    | 297  | VAL  | Mainchain         |
| 7   | Q8    | 298  | SER  | Mainchain         |
| 7   | Q8    | 300  | SER  | Mainchain         |
| 7   | Q8    | 88   | ASN  | Mainchain         |
| 7   | Q8    | 89   | GLY  | Mainchain         |
| 7   | Q8    | 90   | GLY  | Mainchain         |
| 7   | Q8    | 92   | GLY  | Mainchain         |
| 7   | Q8    | 94   | SER  | Mainchain         |
| 1   | R     | 1143 | ALA  | Mainchain         |
| 1   | R     | 1144 | CYS  | Mainchain         |
| 1   | R     | 1146 | ASP  | Mainchain         |
| 1   | R     | 1182 | PRO  | Mainchain         |
| 1   | R     | 1183 | GLU  | Mainchain         |
| 1   | R     | 1184 | GLU  | Mainchain         |
| 1   | R     | 1185 | THR  | Mainchain         |
| 1   | R     | 1186 | THR  | Mainchain         |
| 1   | R     | 1187 | ARG  | Mainchain         |
| 1   | R     | 1188 | TYR  | Mainchain         |
| 1   | R     | 1189 | PRO  | Mainchain         |
| 1   | R     | 1190 | VAL  | Mainchain         |
| 1   | R     | 1191 | LYS  | Mainchain         |
| 1   | R     | 1192 | LYS  | Mainchain         |
| 1   | R     | 1193 | ALA  | Mainchain         |
| 1   | R     | 1194 | ARG  | Mainchain         |
| 1   | R     | 1195 | ARG  | Peptide,Mainchain |
| 1   | R     | 1197 | GLU  | Mainchain         |
| 1   | R     | 1200 | GLN  | Mainchain         |
| 1   | R     | 1201 | LEU  | Mainchain         |
| 1   | R     | 1202 | ARG  | Peptide,Mainchain |
| 1   | R     | 1203 | SER  | Peptide,Mainchain |
| 1   | R     | 1204 | ASN  | Mainchain         |
| 1   | R     | 1205 | ASP  | Mainchain         |
| 1   | R     | 1206 | GLN  | Mainchain         |
| 1   | R     | 1207 | PRO  | Mainchain         |
| 1   | R     | 1208 | LYS  | Mainchain         |
| 1   | R     | 1209 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 1   | R     | 1210 | GLU  | Mainchain         |
| 1   | R     | 1211 | LYS  | Mainchain         |
| 1   | R     | 1293 | CYS  | Mainchain         |
| 1   | R     | 1325 | GLN  | Mainchain         |
| 1   | R     | 1381 | GLU  | Mainchain         |
| 1   | R     | 436  | ARG  | Sidechain         |
| 1   | R     | 47   | ASP  | Peptide           |
| 1   | R     | 480  | PHE  | Sidechain         |
| 1   | R     | 501  | ARG  | Sidechain         |
| 1   | R     | 596  | ARG  | Sidechain         |
| 1   | R     | 605  | TYR  | Peptide           |
| 1   | R     | 801  | PHE  | Sidechain         |
| 1   | R     | 900  | ARG  | Sidechain         |
| 1   | R     | 910  | ARG  | Sidechain         |
| 1   | R16   | 1143 | ALA  | Mainchain         |
| 1   | R16   | 1144 | CYS  | Mainchain         |
| 1   | R16   | 1146 | ASP  | Mainchain         |
| 1   | R16   | 1182 | PRO  | Mainchain         |
| 1   | R16   | 1183 | GLU  | Mainchain         |
| 1   | R16   | 1184 | GLU  | Mainchain         |
| 1   | R16   | 1185 | THR  | Mainchain         |
| 1   | R16   | 1186 | THR  | Mainchain         |
| 1   | R16   | 1187 | ARG  | Mainchain         |
| 1   | R16   | 1188 | TYR  | Mainchain         |
| 1   | R16   | 1189 | PRO  | Mainchain         |
| 1   | R16   | 1190 | VAL  | Mainchain         |
| 1   | R16   | 1191 | LYS  | Mainchain         |
| 1   | R16   | 1192 | LYS  | Mainchain         |
| 1   | R16   | 1193 | ALA  | Mainchain         |
| 1   | R16   | 1194 | ARG  | Mainchain         |
| 1   | R16   | 1195 | ARG  | Peptide,Mainchain |
| 1   | R16   | 1197 | GLU  | Mainchain         |
| 1   | R16   | 1200 | GLN  | Mainchain         |
| 1   | R16   | 1201 | LEU  | Mainchain         |
| 1   | R16   | 1202 | ARG  | Peptide,Mainchain |
| 1   | R16   | 1203 | SER  | Peptide,Mainchain |
| 1   | R16   | 1204 | ASN  | Mainchain         |
| 1   | R16   | 1205 | ASP  | Mainchain         |
| 1   | R16   | 1206 | GLN  | Mainchain         |
| 1   | R16   | 1207 | PRO  | Mainchain         |
| 1   | R16   | 1208 | LYS  | Mainchain         |
| 1   | R16   | 1209 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 1   | R16   | 1210 | GLU  | Mainchain         |
| 1   | R16   | 1211 | LYS  | Mainchain         |
| 1   | R16   | 1293 | CYS  | Mainchain         |
| 1   | R16   | 1325 | GLN  | Mainchain         |
| 1   | R16   | 1381 | GLU  | Mainchain         |
| 1   | R16   | 436  | ARG  | Sidechain         |
| 1   | R16   | 47   | ASP  | Peptide           |
| 1   | R16   | 480  | PHE  | Sidechain         |
| 1   | R16   | 501  | ARG  | Sidechain         |
| 1   | R16   | 596  | ARG  | Sidechain         |
| 1   | R16   | 605  | TYR  | Peptide           |
| 1   | R16   | 801  | PHE  | Sidechain         |
| 1   | R16   | 900  | ARG  | Sidechain         |
| 1   | R16   | 910  | ARG  | Sidechain         |
| 1   | R8    | 1143 | ALA  | Mainchain         |
| 1   | R8    | 1144 | CYS  | Mainchain         |
| 1   | R8    | 1146 | ASP  | Mainchain         |
| 1   | R8    | 1182 | PRO  | Mainchain         |
| 1   | R8    | 1183 | GLU  | Mainchain         |
| 1   | R8    | 1184 | GLU  | Mainchain         |
| 1   | R8    | 1185 | THR  | Mainchain         |
| 1   | R8    | 1186 | THR  | Mainchain         |
| 1   | R8    | 1187 | ARG  | Mainchain         |
| 1   | R8    | 1188 | TYR  | Mainchain         |
| 1   | R8    | 1189 | PRO  | Mainchain         |
| 1   | R8    | 1190 | VAL  | Mainchain         |
| 1   | R8    | 1191 | LYS  | Mainchain         |
| 1   | R8    | 1192 | LYS  | Mainchain         |
| 1   | R8    | 1193 | ALA  | Mainchain         |
| 1   | R8    | 1194 | ARG  | Mainchain         |
| 1   | R8    | 1195 | ARG  | Peptide,Mainchain |
| 1   | R8    | 1197 | GLU  | Mainchain         |
| 1   | R8    | 1200 | GLN  | Mainchain         |
| 1   | R8    | 1201 | LEU  | Mainchain         |
| 1   | R8    | 1202 | ARG  | Peptide,Mainchain |
| 1   | R8    | 1203 | SER  | Peptide,Mainchain |
| 1   | R8    | 1204 | ASN  | Mainchain         |
| 1   | R8    | 1205 | ASP  | Mainchain         |
| 1   | R8    | 1206 | GLN  | Mainchain         |
| 1   | R8    | 1207 | PRO  | Mainchain         |
| 1   | R8    | 1208 | LYS  | Mainchain         |
| 1   | R8    | 1209 | GLY  | Mainchain         |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 1   | R8    | 1210 | GLU  | Mainchain         |
| 1   | R8    | 1211 | LYS  | Mainchain         |
| 1   | R8    | 1293 | CYS  | Mainchain         |
| 1   | R8    | 1325 | GLN  | Mainchain         |
| 1   | R8    | 1381 | GLU  | Mainchain         |
| 1   | R8    | 436  | ARG  | Sidechain         |
| 1   | R8    | 47   | ASP  | Peptide           |
| 1   | R8    | 480  | PHE  | Sidechain         |
| 1   | R8    | 501  | ARG  | Sidechain         |
| 1   | R8    | 596  | ARG  | Sidechain         |
| 1   | R8    | 605  | TYR  | Peptide           |
| 1   | R8    | 801  | PHE  | Sidechain         |
| 1   | R8    | 900  | ARG  | Sidechain         |
| 1   | R8    | 910  | ARG  | Sidechain         |
| 4   | T     | 1    | MET  | Peptide           |
| 4   | T     | 361  | ARG  | Sidechain         |
| 4   | T     | 371  | TYR  | Sidechain         |
| 4   | T     | 386  | HIS  | Sidechain         |
| 4   | T     | 510  | ARG  | Sidechain         |
| 4   | T     | 524  | ARG  | Sidechain         |
| 4   | T     | 547  | LEU  | Peptide           |
| 4   | T16   | 1    | MET  | Peptide           |
| 4   | T16   | 361  | ARG  | Sidechain         |
| 4   | T16   | 371  | TYR  | Sidechain         |
| 4   | T16   | 386  | HIS  | Sidechain         |
| 4   | T16   | 510  | ARG  | Sidechain         |
| 4   | T16   | 524  | ARG  | Sidechain         |
| 4   | T16   | 547  | LEU  | Peptide           |
| 4   | T8    | 1    | MET  | Peptide           |
| 4   | T8    | 361  | ARG  | Sidechain         |
| 4   | T8    | 371  | TYR  | Sidechain         |
| 4   | T8    | 386  | HIS  | Sidechain         |
| 4   | T8    | 510  | ARG  | Sidechain         |
| 4   | T8    | 524  | ARG  | Sidechain         |
| 4   | T8    | 547  | LEU  | Peptide           |
| 13  | V     | 820  | ASP  | Mainchain         |
| 13  | V     | 831  | LYS  | Mainchain         |
| 13  | V     | 833  | ASN  | Mainchain         |
| 13  | V     | 872  | ASP  | Mainchain         |
| 13  | V     | 873  | GLY  | Peptide,Mainchain |
| 13  | V     | 875  | HIS  | Mainchain         |
| 13  | V     | 876  | PRO  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 13  | V     | 877 | VAL  | Mainchain         |
| 13  | V     | 878 | ALA  | Mainchain         |
| 13  | V     | 879 | ARG  | Mainchain         |
| 13  | V     | 880 | ARG  | Peptide,Mainchain |
| 13  | V     | 881 | GLY  | Peptide,Mainchain |
| 13  | V     | 882 | VAL  | Mainchain         |
| 13  | V     | 883 | PRO  | Mainchain         |
| 13  | V     | 884 | ASN  | Mainchain         |
| 13  | V     | 885 | ARG  | Peptide,Mainchain |
| 13  | V     | 886 | SER  | Mainchain         |
| 13  | V     | 887 | ALA  | Mainchain         |
| 13  | V     | 888 | PRO  | Mainchain         |
| 13  | V     | 889 | SER  | Mainchain         |
| 14  | W     | 212 | ARG  | Sidechain         |
| 14  | W     | 338 | GLY  | Peptide           |
| 14  | W     | 339 | ASP  | Peptide           |
| 14  | W     | 592 | ALA  | Mainchain         |
| 14  | W     | 597 | ARG  | Mainchain         |
| 14  | W     | 598 | ILE  | Mainchain         |
| 14  | W     | 600 | PRO  | Mainchain         |
| 14  | W     | 602 | ALA  | Mainchain         |
| 14  | W     | 603 | LEU  | Mainchain         |
| 14  | W     | 70  | ARG  | Sidechain         |
| 14  | W     | 701 | LEU  | Mainchain         |
| 14  | W     | 702 | PRO  | Mainchain         |
| 14  | W     | 703 | GLY  | Mainchain         |
| 14  | W     | 704 | THR  | Mainchain         |
| 14  | W     | 705 | HIS  | Mainchain         |
| 14  | W     | 752 | GLY  | Mainchain         |
| 14  | W     | 757 | ALA  | Mainchain         |
| 14  | W     | 758 | SER  | Mainchain         |
| 14  | W     | 764 | SER  | Peptide           |
| 14  | W     | 765 | LYS  | Mainchain         |
| 14  | W     | 766 | LYS  | Mainchain         |
| 14  | W     | 768 | LEU  | Mainchain         |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | R     | 11593 | 0        | 11503    | 425     | 0            |
| 1   | R16   | 11593 | 0        | 11502    | 207     | 0            |
| 1   | R8    | 11593 | 0        | 11503    | 298     | 0            |
| 2   | M     | 5598  | 0        | 5453     | 470     | 0            |
| 2   | M16   | 5598  | 0        | 5451     | 523     | 0            |
| 2   | M8    | 5598  | 0        | 5449     | 487     | 0            |
| 3   | N     | 2302  | 0        | 2202     | 186     | 0            |
| 3   | N16   | 2302  | 0        | 2202     | 192     | 0            |
| 3   | N8    | 2302  | 0        | 2202     | 185     | 0            |
| 4   | T     | 5498  | 0        | 5401     | 66      | 0            |
| 4   | T16   | 5498  | 0        | 5401     | 68      | 0            |
| 4   | T8    | 5498  | 0        | 5401     | 68      | 0            |
| 5   | P     | 5620  | 0        | 5646     | 488     | 0            |
| 5   | P16   | 5620  | 0        | 5647     | 375     | 0            |
| 5   | P8    | 5620  | 0        | 5647     | 389     | 0            |
| 6   | O     | 2336  | 0        | 2241     | 218     | 0            |
| 6   | O16   | 2336  | 0        | 2243     | 164     | 0            |
| 6   | O8    | 2336  | 0        | 2243     | 181     | 0            |
| 7   | Q     | 2770  | 0        | 2651     | 175     | 0            |
| 7   | Q16   | 2770  | 0        | 2651     | 163     | 0            |
| 7   | Q8    | 2770  | 0        | 2651     | 167     | 0            |
| 8   | L     | 7770  | 0        | 7584     | 103     | 0            |
| 8   | L16   | 7770  | 0        | 7579     | 207     | 0            |
| 8   | L8    | 7770  | 0        | 7583     | 161     | 0            |
| 9   | K     | 5695  | 0        | 5537     | 500     | 0            |
| 9   | K16   | 5696  | 0        | 5544     | 128     | 0            |
| 9   | K8    | 5695  | 0        | 5537     | 493     | 0            |
| 10  | C     | 14402 | 0        | 14575    | 1157    | 0            |
| 10  | C16   | 14529 | 0        | 14695    | 1187    | 0            |
| 10  | C24   | 14529 | 0        | 14696    | 1208    | 0            |
| 10  | C32   | 14529 | 0        | 14697    | 1031    | 0            |
| 10  | C8    | 14177 | 0        | 14346    | 1063    | 0            |
| 11  | A16   | 6472  | 0        | 6473     | 547     | 0            |
| 11  | A24   | 6472  | 0        | 6474     | 496     | 0            |
| 11  | A32   | 6472  | 0        | 6472     | 530     | 0            |
| 11  | A40   | 6472  | 0        | 6474     | 503     | 0            |
| 12  | A     | 5726  | 0        | 5723     | 313     | 0            |
| 12  | A48   | 5752  | 0        | 5745     | 317     | 0            |
| 13  | V     | 1590  | 0        | 1576     | 201     | 0            |
| 14  | W     | 6141  | 0        | 6109     | 391     | 0            |
| 15  | J     | 1504  | 0        | 1487     | 188     | 0            |
| 16  | A8    | 523   | 0        | 517      | 33      | 0            |
| 17  | F     | 213   | 0        | 187      | 41      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 17  | F16   | 213    | 0        | 187      | 40      | 0            |
| 17  | F24   | 213    | 0        | 187      | 39      | 0            |
| 17  | F8    | 213    | 0        | 187      | 40      | 0            |
| 18  | B     | 15417  | 0        | 15672    | 1142    | 0            |
| 18  | B8    | 15417  | 0        | 15674    | 1132    | 0            |
| 19  | 4     | 3413   | 0        | 3328     | 200     | 0            |
| 19  | 48    | 3413   | 0        | 3328     | 214     | 0            |
| 20  | E     | 4057   | 0        | 4120     | 256     | 0            |
| 20  | E8    | 4057   | 0        | 4120     | 272     | 0            |
| 21  | H     | 2023   | 0        | 2068     | 226     | 0            |
| 21  | H16   | 2023   | 0        | 2066     | 194     | 0            |
| 21  | H24   | 2023   | 0        | 2066     | 231     | 0            |
| 21  | H8    | 2023   | 0        | 2066     | 189     | 0            |
| 22  | I     | 1939   | 0        | 1924     | 202     | 0            |
| 22  | I16   | 1939   | 0        | 1924     | 206     | 0            |
| 22  | I24   | 1939   | 0        | 1924     | 200     | 0            |
| 22  | I8    | 1939   | 0        | 1923     | 189     | 0            |
| 23  | J16   | 1601   | 0        | 1575     | 175     | 0            |
| 23  | J24   | 1601   | 0        | 1575     | 203     | 0            |
| 23  | J32   | 1601   | 0        | 1575     | 201     | 0            |
| 23  | J8    | 1601   | 0        | 1575     | 173     | 0            |
| 24  | D     | 11141  | 0        | 11068    | 316     | 0            |
| 24  | D16   | 11141  | 0        | 11074    | 343     | 0            |
| 24  | D24   | 11141  | 0        | 11072    | 147     | 0            |
| 24  | D32   | 11141  | 0        | 11074    | 263     | 0            |
| 24  | D40   | 11141  | 0        | 11072    | 230     | 0            |
| 24  | D8    | 11141  | 0        | 11075    | 152     | 0            |
| All | All   | 402561 | 0        | 400399   | 18966   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (18966) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:B8:1210:CYS:SG | 18:B8:1234:MET:HE1 | 1.23                     | 1.74              |
| 2:M:847:PHE:HB2   | 4:T:656:TRP:CZ3    | 1.17                     | 1.70              |
| 9:K8:1085:TYR:CE1 | 9:K8:1093:SER:HB2  | 1.24                     | 1.68              |
| 10:C:345:MET:HE1  | 10:C:401:ILE:CD1   | 1.19                     | 1.67              |
| 18:B:1210:CYS:SG  | 18:B:1234:MET:HE1  | 1.23                     | 1.67              |
| 20:E:353:ILE:HD13 | 20:E:413:PHE:CD2   | 1.26                     | 1.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:90:PHE:CG     | 18:B8:1788:ILE:HG21  | 1.25                     | 1.65              |
| 11:A32:90:PHE:CB     | 18:B8:1788:ILE:HD13  | 1.22                     | 1.65              |
| 2:M:844:VAL:CG2      | 4:T:660:LEU:HD21     | 1.21                     | 1.64              |
| 10:C32:345:MET:HE1   | 10:C32:401:ILE:CD1   | 1.19                     | 1.64              |
| 20:E8:353:ILE:HD13   | 20:E8:413:PHE:CD2    | 1.26                     | 1.64              |
| 10:C16:1285:VAL:CG2  | 10:C16:1738:MET:HE2  | 1.16                     | 1.64              |
| 11:A32:212:LYS:CE    | 11:A32:585:MET:HE1   | 1.19                     | 1.63              |
| 10:C8:453:LEU:HD22   | 10:C8:459:LEU:CD2    | 1.28                     | 1.63              |
| 11:A40:212:LYS:CE    | 11:A40:585:MET:HE1   | 1.19                     | 1.62              |
| 2:M8:847:PHE:HB2     | 4:T8:656:TRP:CZ3     | 1.17                     | 1.61              |
| 5:P8:614:VAL:HB      | 5:P8:629:ARG:CZ      | 1.20                     | 1.61              |
| 10:C24:1285:VAL:CG2  | 10:C24:1738:MET:HE2  | 1.16                     | 1.61              |
| 10:C32:453:LEU:HD22  | 10:C32:459:LEU:CD2   | 1.28                     | 1.61              |
| 11:A16:212:LYS:CE    | 11:A16:585:MET:HE1   | 1.19                     | 1.61              |
| 2:M16:847:PHE:HB2    | 4:T16:656:TRP:CZ3    | 1.17                     | 1.61              |
| 10:C24:1285:VAL:HG21 | 10:C24:1738:MET:CE   | 1.28                     | 1.60              |
| 11:A16:90:PHE:CG     | 18:B:1788:ILE:HG21   | 1.24                     | 1.60              |
| 9:K:1085:TYR:CE1     | 9:K:1093:SER:HB2     | 1.24                     | 1.60              |
| 10:C16:390:HIS:CD2   | 10:C16:452:LEU:HB3   | 1.34                     | 1.60              |
| 10:C16:1548:ILE:CD1  | 24:D8:1407:PHE:CZ    | 1.81                     | 1.60              |
| 11:A32:90:PHE:HB2    | 18:B8:1788:ILE:CD1   | 1.24                     | 1.60              |
| 1:R8:1265:PHE:CE2    | 1:R8:1269:LEU:HD11   | 1.37                     | 1.60              |
| 10:C:453:LEU:HD22    | 10:C:459:LEU:CD2     | 1.28                     | 1.60              |
| 10:C32:1348:LEU:CD1  | 10:C32:1359:ILE:HD11 | 1.15                     | 1.59              |
| 2:M8:669:ALA:CB      | 2:M8:684:GLN:CG      | 1.77                     | 1.59              |
| 10:C24:453:LEU:HD22  | 10:C24:459:LEU:CD2   | 1.28                     | 1.59              |
| 8:L:601:HIS:CE1      | 8:L:631:LEU:HD22     | 1.33                     | 1.59              |
| 20:E:353:ILE:CD1     | 20:E:413:PHE:CD2     | 1.85                     | 1.59              |
| 10:C16:345:MET:HE1   | 10:C16:401:ILE:CD1   | 1.19                     | 1.59              |
| 10:C24:1548:ILE:HD11 | 24:D24:1407:PHE:CZ   | 1.21                     | 1.59              |
| 2:M16:540:TYR:CE1    | 2:M16:555:LEU:HD23   | 1.34                     | 1.58              |
| 10:C24:390:HIS:HB3   | 10:C24:452:LEU:CG    | 1.31                     | 1.58              |
| 10:C24:1548:ILE:HD11 | 24:D24:1407:PHE:CE2  | 1.32                     | 1.58              |
| 13:V:902:MET:HE1     | 14:W:777:LEU:CD2     | 1.26                     | 1.58              |
| 5:P:109:ILE:HG12     | 14:W:18:PRO:CG       | 1.29                     | 1.58              |
| 10:C:345:MET:CE      | 10:C:401:ILE:HD11    | 1.34                     | 1.58              |
| 10:C8:345:MET:HE1    | 10:C8:401:ILE:CD1    | 1.19                     | 1.58              |
| 11:A24:468:VAL:HG22  | 24:D16:1103:LEU:CD1  | 1.19                     | 1.58              |
| 10:C24:1348:LEU:CD1  | 10:C24:1359:ILE:HD11 | 1.15                     | 1.58              |
| 24:D:409:LEU:HD13    | 24:D16:746:ALA:CA    | 1.22                     | 1.58              |
| 24:D40:839:GLU:HB3   | 24:D40:971:HIS:CE1   | 1.39                     | 1.58              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 12:A48:212:LYS:CE    | 12:A48:585:MET:HE1   | 1.19                     | 1.58              |
| 10:C24:345:MET:HE1   | 10:C24:401:ILE:CD1   | 1.19                     | 1.58              |
| 5:P16:101:LEU:CD2    | 5:P16:133:TYR:CZ     | 1.88                     | 1.57              |
| 9:K:792:LEU:HD12     | 9:K:864:ILE:CD1      | 1.24                     | 1.57              |
| 10:C:1348:LEU:CD1    | 10:C:1359:ILE:HD11   | 1.15                     | 1.57              |
| 10:C32:1285:VAL:HG21 | 10:C32:1738:MET:CE   | 1.28                     | 1.57              |
| 2:M16:540:TYR:CD1    | 2:M16:555:LEU:CD2    | 1.85                     | 1.57              |
| 2:M16:844:VAL:CG2    | 4:T16:660:LEU:HD21   | 1.19                     | 1.57              |
| 10:C:345:MET:CE      | 10:C:401:ILE:CD1     | 1.81                     | 1.57              |
| 10:C:1285:VAL:HG21   | 10:C:1738:MET:CE     | 1.28                     | 1.57              |
| 10:C8:1285:VAL:HG21  | 10:C8:1738:MET:CE    | 1.28                     | 1.57              |
| 18:B8:1439:LYS:CE    | 24:D32:1257:ASN:HB3  | 1.31                     | 1.57              |
| 8:L16:851:PRO:HG2    | 9:K16:1283:PRO:CB    | 1.21                     | 1.57              |
| 10:C16:1285:VAL:HG21 | 10:C16:1738:MET:CE   | 1.28                     | 1.57              |
| 11:A24:212:LYS:CE    | 11:A24:585:MET:HE1   | 1.19                     | 1.56              |
| 10:C24:1453:ARG:HH22 | 24:D24:1150:GLY:CA   | 1.02                     | 1.56              |
| 10:C:1285:VAL:CG2    | 10:C:1738:MET:HE2    | 1.16                     | 1.56              |
| 18:B8:195:MET:HE2    | 18:B8:199:LEU:CD2    | 1.29                     | 1.56              |
| 11:A32:90:PHE:CD1    | 18:B8:1788:ILE:HG21  | 1.39                     | 1.56              |
| 18:B8:712:PRO:HG2    | 18:B8:759:MET:CE     | 1.33                     | 1.56              |
| 8:L16:1071:LEU:HD11  | 9:K16:1284:MET:SD    | 1.43                     | 1.55              |
| 10:C8:345:MET:CE     | 10:C8:401:ILE:HD11   | 1.34                     | 1.55              |
| 10:C32:1285:VAL:CG2  | 10:C32:1738:MET:HE2  | 1.16                     | 1.55              |
| 12:A:212:LYS:CE      | 12:A:585:MET:HE1     | 1.19                     | 1.55              |
| 18:B:195:MET:HE2     | 18:B:199:LEU:CD2     | 1.29                     | 1.55              |
| 2:M8:669:ALA:CB      | 2:M8:684:GLN:HG3     | 1.10                     | 1.55              |
| 2:M8:844:VAL:CG2     | 4:T8:660:LEU:HD21    | 1.19                     | 1.55              |
| 10:C8:1285:VAL:CG2   | 10:C8:1738:MET:HE2   | 1.16                     | 1.55              |
| 10:C8:1348:LEU:CD1   | 10:C8:1359:ILE:HD11  | 1.15                     | 1.55              |
| 10:C16:1348:LEU:CD1  | 10:C16:1359:ILE:HD11 | 1.15                     | 1.55              |
| 8:L16:851:PRO:CG     | 9:K16:1283:PRO:HB3   | 1.11                     | 1.55              |
| 10:C16:453:LEU:HD22  | 10:C16:459:LEU:CD2   | 1.28                     | 1.55              |
| 19:4:250:ILE:CG2     | 20:E:165:ARG:HH22    | 1.20                     | 1.55              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:CD2    | 1.85                     | 1.55              |
| 10:C24:345:MET:CE    | 10:C24:401:ILE:CD1   | 1.81                     | 1.54              |
| 10:C16:345:MET:CE    | 10:C16:401:ILE:HD11  | 1.34                     | 1.54              |
| 18:B:712:PRO:HG2     | 18:B:759:MET:CE      | 1.33                     | 1.54              |
| 10:C24:345:MET:CE    | 10:C24:401:ILE:HD11  | 1.34                     | 1.53              |
| 1:R8:1059:ILE:CG2    | 24:D40:1435:ARG:NH2  | 1.72                     | 1.53              |
| 5:P:322:CYS:SG       | 13:V:763:LYS:HE2     | 1.46                     | 1.53              |
| 2:M:847:PHE:CB       | 4:T:656:TRP:CZ3      | 1.91                     | 1.53              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:345:MET:CE    | 10:C16:401:ILE:CD1   | 1.81                     | 1.53              |
| 10:C32:453:LEU:CD2   | 10:C32:459:LEU:HD21  | 1.37                     | 1.53              |
| 10:C16:1548:ILE:HD11 | 24:D8:1407:PHE:CE2   | 1.41                     | 1.53              |
| 10:C:153:ALA:HB1     | 24:D:1403:LEU:CD1    | 1.38                     | 1.53              |
| 19:48:250:ILE:CG2    | 20:E8:165:ARG:HH22   | 1.20                     | 1.53              |
| 3:N8:162:THR:HG23    | 3:N8:168:VAL:CG2     | 1.36                     | 1.52              |
| 10:C8:453:LEU:CD2    | 10:C8:459:LEU:HD21   | 1.37                     | 1.52              |
| 10:C8:345:MET:CE     | 10:C8:401:ILE:CD1    | 1.81                     | 1.52              |
| 11:A40:468:VAL:HG22  | 24:D32:1103:LEU:CD1  | 1.33                     | 1.52              |
| 11:A16:91:GLU:CB     | 18:B:1112:LYS:NZ     | 1.70                     | 1.52              |
| 2:M8:351:ALA:HB1     | 8:L8:219:ILE:CG2     | 1.38                     | 1.51              |
| 3:N16:162:THR:HG23   | 3:N16:168:VAL:CG2    | 1.36                     | 1.51              |
| 18:B:1575:GLN:HE21   | 24:D16:1403:LEU:CD2  | 1.20                     | 1.51              |
| 3:N:162:THR:HG23     | 3:N:168:VAL:CG2      | 1.36                     | 1.51              |
| 20:E8:340:GLY:C      | 20:E8:341:TYR:N      | 1.67                     | 1.51              |
| 10:C32:643:LEU:HD11  | 10:C32:679:ARG:NH1   | 1.19                     | 1.51              |
| 8:L8:976:LEU:CD2     | 9:K8:1004:ARG:HD3    | 1.37                     | 1.51              |
| 11:A24:468:VAL:CG2   | 24:D16:1103:LEU:HD12 | 1.37                     | 1.51              |
| 2:M8:847:PHE:CB      | 4:T8:656:TRP:CZ3     | 1.91                     | 1.51              |
| 10:C16:407:LYS:HE3   | 10:C16:465:PHE:CZ    | 1.45                     | 1.51              |
| 3:N8:162:THR:CG2     | 3:N8:168:VAL:HG23    | 1.41                     | 1.50              |
| 2:M16:847:PHE:CB     | 4:T16:656:TRP:CZ3    | 1.91                     | 1.50              |
| 11:A16:676:TYR:CZ    | 24:D16:1395:SER:HA   | 1.44                     | 1.50              |
| 18:B8:786:ASP:CG     | 24:D32:1066:VAL:HG22 | 1.32                     | 1.50              |
| 10:C24:453:LEU:CD2   | 10:C24:459:LEU:HD21  | 1.37                     | 1.50              |
| 10:C24:407:LYS:HE3   | 10:C24:465:PHE:CZ    | 1.45                     | 1.50              |
| 20:E:340:GLY:C       | 20:E:341:TYR:N       | 1.67                     | 1.50              |
| 2:M8:730:GLU:HG2     | 8:L16:504:GLN:NE2    | 1.18                     | 1.50              |
| 10:C:670:GLU:C       | 10:C:671:LYS:N       | 1.67                     | 1.50              |
| 10:C32:345:MET:CE    | 10:C32:401:ILE:CD1   | 1.81                     | 1.50              |
| 10:C32:407:LYS:HE3   | 10:C32:465:PHE:CZ    | 1.45                     | 1.50              |
| 10:C:453:LEU:CD2     | 10:C:459:LEU:HD21    | 1.38                     | 1.49              |
| 10:C8:670:GLU:C      | 10:C8:671:LYS:N      | 1.67                     | 1.49              |
| 20:E8:434:TRP:NE1    | 24:D40:72:GLU:CB     | 1.71                     | 1.49              |
| 2:M8:730:GLU:CG      | 8:L16:504:GLN:NE2    | 1.70                     | 1.49              |
| 2:M16:231:ARG:NE     | 2:M16:299:GLY:HA2    | 1.22                     | 1.49              |
| 10:C16:453:LEU:CD2   | 10:C16:459:LEU:HD21  | 1.37                     | 1.49              |
| 10:C16:670:GLU:C     | 10:C16:671:LYS:N     | 1.67                     | 1.49              |
| 11:A40:803:PRO:HB3   | 24:D24:1401:LEU:CD1  | 1.43                     | 1.49              |
| 1:R8:1449:TRP:CZ3    | 2:M8:160:LEU:HD12    | 1.47                     | 1.49              |
| 10:C32:670:GLU:C     | 10:C32:671:LYS:N     | 1.67                     | 1.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:R:1428:VAL:HG21   | 6:O:165:LYS:CE      | 1.43                     | 1.48              |
| 14:W:513:SER:C      | 14:W:607:ARG:HH12   | 1.18                     | 1.48              |
| 21:H8:269:PHE:CD1   | 22:I8:205:ARG:NH1   | 1.81                     | 1.48              |
| 21:H16:269:PHE:CD1  | 22:I16:205:ARG:NH1  | 1.81                     | 1.48              |
| 10:C24:670:GLU:C    | 10:C24:671:LYS:N    | 1.67                     | 1.48              |
| 14:W:711:ARG:NH1    | 10:C8:1609:ASP:HB2  | 1.28                     | 1.48              |
| 14:W:584:CYS:SG     | 15:J:573:LYS:HE3    | 1.52                     | 1.48              |
| 5:P:57:PRO:HB2      | 6:O:29:LEU:CD1      | 1.41                     | 1.47              |
| 5:P8:57:PRO:HB2     | 6:O8:29:LEU:CD1     | 1.41                     | 1.47              |
| 8:L8:976:LEU:CD2    | 9:K8:1004:ARG:CD    | 1.90                     | 1.47              |
| 11:A40:326:TYR:CE1  | 17:F16:77:TYR:HB2   | 1.49                     | 1.47              |
| 13:V:844:MET:CG     | 10:C8:1502:ARG:NH2  | 1.78                     | 1.47              |
| 11:A16:326:TYR:CE1  | 17:F8:77:TYR:HB2    | 1.49                     | 1.47              |
| 11:A32:90:PHE:CD1   | 18:B8:1788:ILE:CG2  | 1.95                     | 1.47              |
| 11:A32:326:TYR:CE1  | 17:F24:77:TYR:HB2   | 1.49                     | 1.47              |
| 2:M8:417:ARG:HB3    | 8:L8:298:PHE:CE2    | 1.47                     | 1.47              |
| 11:A24:326:TYR:CE1  | 17:F:77:TYR:HB2     | 1.49                     | 1.47              |
| 14:W:715:ASP:HA     | 10:C8:1568:ARG:NH1  | 1.20                     | 1.47              |
| 1:R:1449:TRP:CZ3    | 2:M:160:LEU:HD12    | 1.47                     | 1.47              |
| 1:R16:1269:LEU:HD13 | 5:P16:684:ARG:CG    | 1.42                     | 1.47              |
| 7:Q8:124:PHE:HD1    | 7:Q8:125:TYR:CE2    | 1.32                     | 1.47              |
| 7:Q16:124:PHE:HD1   | 7:Q16:125:TYR:CE2   | 1.32                     | 1.47              |
| 9:K:1085:TYR:CE1    | 9:K:1093:SER:CB     | 1.98                     | 1.47              |
| 1:R:1425:PRO:HA     | 6:O:165:LYS:NZ      | 1.17                     | 1.46              |
| 5:P:152:ILE:HG21    | 14:W:762:GLN:NE2    | 1.28                     | 1.46              |
| 7:Q:124:PHE:HD1     | 7:Q:125:TYR:CE2     | 1.32                     | 1.46              |
| 10:C24:1453:ARG:NH2 | 24:D24:1150:GLY:HA3 | 1.21                     | 1.46              |
| 2:M:847:PHE:HB2     | 4:T:656:TRP:CH2     | 1.49                     | 1.46              |
| 5:P16:57:PRO:HB2    | 6:O16:29:LEU:CD1    | 1.41                     | 1.46              |
| 14:W:515:CYS:HB3    | 14:W:604:PRO:CD     | 1.09                     | 1.46              |
| 21:H8:231:HIS:HD2   | 23:J8:596:GLN:NE2   | 1.08                     | 1.46              |
| 3:N:162:THR:CG2     | 3:N:168:VAL:HG23    | 1.41                     | 1.45              |
| 20:E8:352:PHE:CE1   | 20:E8:451:ILE:HD13  | 1.48                     | 1.45              |
| 6:O16:179:LYS:CD    | 6:O16:183:GLN:OE1   | 1.64                     | 1.45              |
| 18:B:195:MET:CE     | 18:B:199:LEU:HD23   | 1.43                     | 1.45              |
| 20:E:352:PHE:CE1    | 20:E:451:ILE:HD13   | 1.48                     | 1.45              |
| 21:H16:312:GLN:HG2  | 21:H16:316:ILE:CD1  | 1.46                     | 1.45              |
| 24:D:308:ASN:ND2    | 24:D16:753:ARG:HE   | 1.06                     | 1.45              |
| 2:M8:417:ARG:CB     | 8:L8:298:PHE:HE2    | 1.28                     | 1.45              |
| 9:K:792:LEU:CD1     | 9:K:864:ILE:CD1     | 1.95                     | 1.45              |
| 1:R16:1449:TRP:CZ3  | 2:M16:160:LEU:HD12  | 1.47                     | 1.45              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 2:M16:540:TYR:CE1  | 2:M16:555:LEU:CD2    | 1.93                     | 1.45              |
| 10:C:153:ALA:CB    | 24:D:1403:LEU:HG     | 1.45                     | 1.45              |
| 2:M16:847:PHE:HB2  | 4:T16:656:TRP:CH2    | 1.49                     | 1.44              |
| 11:A16:90:PHE:HB3  | 18:B:1800:ARG:NH2    | 1.29                     | 1.44              |
| 18:B:1575:GLN:NE2  | 24:D16:1403:LEU:HD23 | 1.32                     | 1.44              |
| 18:B8:195:MET:CE   | 18:B8:199:LEU:HD23   | 1.43                     | 1.44              |
| 21:H:269:PHE:CD1   | 22:I:205:ARG:NH1     | 1.81                     | 1.44              |
| 6:O:179:LYS:CD     | 6:O:183:GLN:OE1      | 1.64                     | 1.44              |
| 10:C16:1664:SER:CA | 10:C24:1568:ARG:HH21 | 1.29                     | 1.44              |
| 21:H24:269:PHE:CD1 | 22:I24:205:ARG:NH1   | 1.81                     | 1.44              |
| 18:B:1529:GLU:OE2  | 24:D16:1415:LEU:CD1  | 1.65                     | 1.44              |
| 2:M8:847:PHE:HB2   | 4:T8:656:TRP:CH2     | 1.49                     | 1.43              |
| 9:K:916:LYS:HG2    | 9:K:919:MET:CE       | 1.46                     | 1.43              |
| 11:A16:90:PHE:CE2  | 18:B:1788:ILE:HG23   | 1.50                     | 1.43              |
| 3:N:162:THR:CG2    | 3:N:168:VAL:CG2      | 1.92                     | 1.43              |
| 3:N16:162:THR:CG2  | 3:N16:168:VAL:HG23   | 1.41                     | 1.43              |
| 11:A16:91:GLU:HB3  | 18:B:1112:LYS:CE     | 1.48                     | 1.43              |
| 21:H:312:GLN:HG2   | 21:H:316:ILE:CD1     | 1.47                     | 1.43              |
| 24:D40:873:ARG:NH1 | 24:D40:884:ASP:HB3   | 1.25                     | 1.43              |
| 11:A32:560:MET:CE  | 11:A32:615:GLN:HE22  | 1.31                     | 1.43              |
| 3:N8:162:THR:CG2   | 3:N8:168:VAL:CG2     | 1.92                     | 1.43              |
| 11:A24:212:LYS:CE  | 11:A24:585:MET:CE    | 1.97                     | 1.43              |
| 21:H:231:HIS:HD2   | 23:J32:596:GLN:NE2   | 1.08                     | 1.43              |
| 10:C32:345:MET:CE  | 10:C32:401:ILE:HD11  | 1.34                     | 1.43              |
| 9:K8:1085:TYR:CE1  | 9:K8:1093:SER:CB     | 1.98                     | 1.43              |
| 11:A40:212:LYS:CE  | 11:A40:585:MET:CE    | 1.97                     | 1.43              |
| 12:A:212:LYS:CE    | 12:A:585:MET:CE      | 1.97                     | 1.43              |
| 21:H8:312:GLN:HG2  | 21:H8:316:ILE:CD1    | 1.46                     | 1.43              |
| 21:H16:231:HIS:HD2 | 23:J16:596:GLN:NE2   | 1.07                     | 1.43              |
| 5:P:109:ILE:CG1    | 14:W:18:PRO:CG       | 1.95                     | 1.42              |
| 11:A16:445:ASN:CB  | 17:F8:65:ARG:NH1     | 1.82                     | 1.42              |
| 18:B8:786:ASP:OD2  | 24:D32:1066:VAL:CG2  | 1.64                     | 1.42              |
| 11:A24:645:GLU:CG  | 24:D16:867:ASP:OD1   | 1.66                     | 1.42              |
| 10:C24:1699:LYS:NZ | 23:J24:722:LEU:HD22  | 1.32                     | 1.42              |
| 11:A16:90:PHE:CD1  | 18:B:1788:ILE:HG21   | 1.53                     | 1.42              |
| 11:A32:90:PHE:CG   | 18:B8:1788:ILE:CG2   | 1.96                     | 1.42              |
| 18:B8:786:ASP:OD1  | 24:D32:1066:VAL:CG1  | 1.65                     | 1.42              |
| 1:R8:1266:THR:HA   | 5:P8:684:ARG:NH2     | 1.24                     | 1.42              |
| 11:A24:560:MET:CE  | 11:A24:615:GLN:HE22  | 1.31                     | 1.42              |
| 11:A32:445:ASN:CB  | 17:F24:65:ARG:NH1    | 1.82                     | 1.42              |
| 2:M16:672:TYR:CB   | 2:M16:680:LYS:HD2    | 1.48                     | 1.42              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 12:A:642:GLY:HA3     | 12:A:685:ARG:CZ     | 1.49                     | 1.42              |
| 11:A16:212:LYS:CE    | 11:A16:585:MET:CE   | 1.97                     | 1.42              |
| 18:B8:1256:THR:CG2   | 24:D32:1238:GLU:HG3 | 1.47                     | 1.42              |
| 23:J32:718:GLN:NE2   | 23:J32:737:TRP:CZ3  | 1.88                     | 1.42              |
| 21:H24:312:GLN:HG2   | 21:H24:316:ILE:CD1  | 1.46                     | 1.42              |
| 10:C32:407:LYS:CD    | 10:C32:465:PHE:HZ   | 1.33                     | 1.42              |
| 2:M16:417:ARG:HD3    | 8:L16:298:PHE:CD2   | 1.54                     | 1.42              |
| 2:M16:428:SER:CB     | 8:L16:355:SER:OG    | 1.64                     | 1.42              |
| 2:M16:672:TYR:CD1    | 2:M16:680:LYS:NZ    | 1.82                     | 1.42              |
| 9:K:743:ARG:NH1      | 9:K:772:TYR:HE1     | 1.14                     | 1.42              |
| 10:C:407:LYS:CD      | 10:C:465:PHE:HZ     | 1.33                     | 1.42              |
| 10:C:979:MET:HE3     | 10:C:1028:ILE:CG2   | 1.47                     | 1.42              |
| 24:D:405:GLN:OE1     | 24:D16:10:ARG:CD    | 1.64                     | 1.42              |
| 24:D:405:GLN:CG      | 24:D16:10:ARG:NH1   | 1.82                     | 1.42              |
| 9:K:719:GLY:C        | 9:K:720:SER:N       | 1.74                     | 1.41              |
| 12:A:560:MET:CE      | 12:A:615:GLN:HE22   | 1.31                     | 1.41              |
| 11:A32:91:GLU:HB2    | 18:B8:1112:LYS:NZ   | 1.30                     | 1.41              |
| 23:J24:718:GLN:NE2   | 23:J24:737:TRP:CZ3  | 1.88                     | 1.41              |
| 2:M:762:LEU:HB2      | 2:M:813:ASN:ND2     | 1.26                     | 1.41              |
| 2:M16:231:ARG:CD     | 2:M16:299:GLY:HA3   | 1.51                     | 1.41              |
| 6:O8:179:LYS:CD      | 6:O8:183:GLN:OE1    | 1.64                     | 1.41              |
| 10:C24:407:LYS:CD    | 10:C24:465:PHE:HZ   | 1.33                     | 1.41              |
| 11:A32:212:LYS:CE    | 11:A32:585:MET:CE   | 1.97                     | 1.41              |
| 8:L:605:MET:SD       | 8:L:631:LEU:HD11    | 1.59                     | 1.41              |
| 21:H24:231:HIS:HD2   | 23:J24:596:GLN:NE2  | 1.08                     | 1.41              |
| 2:M16:762:LEU:HB2    | 2:M16:813:ASN:ND2   | 1.26                     | 1.41              |
| 10:C16:1548:ILE:HD11 | 24:D8:1407:PHE:CZ   | 0.89                     | 1.41              |
| 20:E8:432:ILE:CD1    | 24:D40:72:GLU:HG3   | 1.49                     | 1.41              |
| 22:I8:196:VAL:HA     | 23:J8:620:MET:CE    | 1.49                     | 1.41              |
| 2:M:428:SER:CB       | 8:L:355:SER:HG      | 1.34                     | 1.41              |
| 7:Q:341:GLN:CG       | 10:C8:751:ARG:HH12  | 1.32                     | 1.41              |
| 5:P16:105:ARG:NH2    | 5:P16:133:TYR:CD1   | 1.76                     | 1.41              |
| 10:C:643:LEU:HD11    | 10:C:679:ARG:NH1    | 1.19                     | 1.41              |
| 23:J16:718:GLN:NE2   | 23:J16:737:TRP:CZ3  | 1.88                     | 1.41              |
| 5:P:600:PHE:CD2      | 5:P:638:SER:CB      | 2.03                     | 1.40              |
| 10:C16:407:LYS:CD    | 10:C16:465:PHE:HZ   | 1.33                     | 1.40              |
| 2:M8:762:LEU:HB2     | 2:M8:813:ASN:ND2    | 1.26                     | 1.40              |
| 9:K8:578:THR:CG2     | 9:K8:616:ARG:NH2    | 1.84                     | 1.40              |
| 5:P:607:PHE:CE1      | 5:P:633:LEU:HD12    | 1.52                     | 1.40              |
| 9:K:578:THR:CG2      | 9:K:616:ARG:NH2     | 1.83                     | 1.40              |
| 11:A24:445:ASN:CB    | 17:F:65:ARG:NH1     | 1.82                     | 1.40              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 13:V:790:GLN:NE2     | 14:W:674:GLN:HE22   | 1.10                     | 1.40              |
| 10:C8:1285:VAL:CG2   | 10:C8:1738:MET:CE   | 1.88                     | 1.40              |
| 24:D:308:ASN:ND2     | 24:D16:753:ARG:NE   | 1.68                     | 1.40              |
| 12:A48:212:LYS:CE    | 12:A48:585:MET:CE   | 1.97                     | 1.40              |
| 1:R:1269:LEU:HD13    | 5:P:684:ARG:CG      | 1.50                     | 1.40              |
| 9:K8:719:GLY:C       | 9:K8:720:SER:N      | 1.74                     | 1.40              |
| 10:C16:1453:ARG:HH22 | 24:D8:1150:GLY:CA   | 1.32                     | 1.40              |
| 11:A16:560:MET:CE    | 11:A16:615:GLN:HE22 | 1.31                     | 1.40              |
| 21:H24:231:HIS:CD2   | 23:J24:596:GLN:NE2  | 1.90                     | 1.40              |
| 12:A48:560:MET:CE    | 12:A48:615:GLN:HE22 | 1.31                     | 1.40              |
| 9:K8:743:ARG:NH1     | 9:K8:772:TYR:HE1    | 1.14                     | 1.40              |
| 10:C24:390:HIS:CB    | 10:C24:452:LEU:HG   | 1.49                     | 1.40              |
| 11:A40:560:MET:CE    | 11:A40:615:GLN:HE22 | 1.31                     | 1.40              |
| 18:B:1110:LEU:CD1    | 21:H:323:TYR:OH     | 1.70                     | 1.40              |
| 20:E8:434:TRP:HE1    | 24:D40:72:GLU:CB    | 1.31                     | 1.40              |
| 23:J8:718:GLN:NE2    | 23:J8:737:TRP:CZ3   | 1.88                     | 1.40              |
| 1:R:1075:LYS:CE      | 5:P:713:LEU:O       | 1.70                     | 1.39              |
| 11:A40:445:ASN:CB    | 17:F16:65:ARG:NH1   | 1.82                     | 1.39              |
| 3:N16:162:THR:CG2    | 3:N16:168:VAL:CG2   | 1.92                     | 1.39              |
| 11:A16:676:TYR:OH    | 24:D16:1395:SER:CA  | 1.69                     | 1.39              |
| 21:H8:231:HIS:CD2    | 23:J8:596:GLN:NE2   | 1.90                     | 1.39              |
| 22:I16:196:VAL:HA    | 23:J16:620:MET:CE   | 1.49                     | 1.39              |
| 1:R16:1269:LEU:CD1   | 5:P16:684:ARG:HG2   | 1.47                     | 1.39              |
| 14:W:586:ILE:CD1     | 15:J:569:ALA:HA     | 1.51                     | 1.39              |
| 10:C32:1285:VAL:CG2  | 10:C32:1738:MET:CE  | 1.88                     | 1.39              |
| 11:A16:90:PHE:CB     | 18:B:1788:ILE:HD13  | 1.49                     | 1.39              |
| 22:I:196:VAL:HA      | 23:J32:620:MET:CE   | 1.49                     | 1.39              |
| 21:H:231:HIS:CD2     | 23:J32:596:GLN:NE2  | 1.90                     | 1.39              |
| 10:C32:407:LYS:CE    | 10:C32:465:PHE:CZ   | 2.05                     | 1.39              |
| 1:R:1424:LYS:NZ      | 6:O:105:ASN:ND2     | 1.71                     | 1.38              |
| 5:P:109:ILE:CG1      | 14:W:18:PRO:HG3     | 1.50                     | 1.38              |
| 11:A24:445:ASN:HB3   | 17:F:65:ARG:NH1     | 1.07                     | 1.38              |
| 11:A40:445:ASN:HB3   | 17:F16:65:ARG:NH1   | 1.07                     | 1.38              |
| 5:P:322:CYS:SG       | 13:V:763:LYS:CE     | 2.10                     | 1.38              |
| 5:P:401:ARG:CD       | 5:P:414:VAL:HG21    | 1.51                     | 1.38              |
| 8:L8:270:LEU:CD2     | 12:A48:155:SER:HB2  | 1.54                     | 1.38              |
| 10:C:110:ARG:NH1     | 10:C:118:LEU:HD11   | 1.37                     | 1.38              |
| 2:M16:231:ARG:CD     | 2:M16:299:GLY:CA    | 2.01                     | 1.38              |
| 2:M16:544:LEU:HD21   | 2:M16:586:ALA:CB    | 1.50                     | 1.38              |
| 10:C24:1708:ARG:CZ   | 21:H24:279:GLU:CD   | 1.78                     | 1.38              |
| 19:48:252:ARG:HG3    | 19:48:281:TRP:CH2   | 1.57                     | 1.38              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I24:196:VAL:HA    | 23:J24:620:MET:CE    | 1.49                     | 1.38              |
| 11:A16:90:PHE:CB     | 18:B:1800:ARG:HH21   | 1.34                     | 1.38              |
| 11:A32:91:GLU:CB     | 18:B8:1112:LYS:NZ    | 1.84                     | 1.38              |
| 18:B:712:PRO:CG      | 18:B:759:MET:CE      | 2.01                     | 1.38              |
| 2:M8:669:ALA:HB2     | 2:M8:684:GLN:CD      | 1.46                     | 1.37              |
| 2:M16:672:TYR:CG     | 2:M16:680:LYS:NZ     | 1.90                     | 1.37              |
| 14:W:517:GLU:N       | 14:W:605:ASN:CA      | 1.74                     | 1.37              |
| 18:B:712:PRO:CG      | 18:B:759:MET:HE1     | 1.55                     | 1.37              |
| 23:J32:686:MET:HE1   | 23:J32:694:ARG:CZ    | 1.52                     | 1.37              |
| 11:A24:362:ARG:HD2   | 11:A24:366:ARG:NH2   | 1.40                     | 1.37              |
| 10:C24:407:LYS:CE    | 10:C24:465:PHE:CZ    | 2.05                     | 1.37              |
| 11:A40:362:ARG:HD2   | 11:A40:366:ARG:NH2   | 1.40                     | 1.37              |
| 21:H16:231:HIS:CD2   | 23:J16:596:GLN:NE2   | 1.89                     | 1.37              |
| 10:C16:407:LYS:CE    | 10:C16:465:PHE:CZ    | 2.05                     | 1.37              |
| 10:C24:1814:LYS:NZ   | 23:J24:738:MET:HB3   | 1.33                     | 1.37              |
| 11:A40:803:PRO:CB    | 24:D24:1401:LEU:HD12 | 1.53                     | 1.37              |
| 2:M16:544:LEU:CD2    | 2:M16:586:ALA:HB1    | 1.55                     | 1.37              |
| 5:P:600:PHE:CE2      | 5:P:638:SER:CB       | 2.05                     | 1.37              |
| 5:P8:614:VAL:CB      | 5:P8:629:ARG:CZ      | 2.01                     | 1.37              |
| 14:W:711:ARG:CD      | 10:C8:1609:ASP:OD2   | 1.71                     | 1.37              |
| 11:A16:90:PHE:HB2    | 18:B:1788:ILE:CD1    | 1.53                     | 1.37              |
| 18:B:686:LEU:HD13    | 18:B:790:ASP:OD2     | 1.25                     | 1.37              |
| 24:D:409:LEU:CD1     | 24:D16:746:ALA:HA    | 1.55                     | 1.37              |
| 13:V:844:MET:HG2     | 10:C8:1502:ARG:NH2   | 1.04                     | 1.36              |
| 18:B8:712:PRO:CG     | 18:B8:759:MET:CE     | 2.01                     | 1.36              |
| 23:J8:686:MET:HE1    | 23:J8:694:ARG:CZ     | 1.52                     | 1.36              |
| 2:M16:414:GLY:HA2    | 8:L16:401:LYS:NZ     | 1.38                     | 1.36              |
| 14:W:590:LEU:HD11    | 14:W:641:GLU:OE2     | 1.20                     | 1.36              |
| 23:J24:686:MET:HE1   | 23:J24:694:ARG:CZ    | 1.52                     | 1.36              |
| 10:C8:110:ARG:NH1    | 10:C8:118:LEU:HD11   | 1.37                     | 1.36              |
| 18:B:1110:LEU:CD2    | 21:H:326:GLY:HA2     | 1.55                     | 1.36              |
| 9:K8:635:ALA:CB      | 9:K8:655:GLN:HE22    | 1.39                     | 1.36              |
| 10:C16:1545:ARG:NH2  | 11:A24:672:GLU:OE2   | 1.58                     | 1.36              |
| 10:C24:1548:ILE:CD1  | 24:D24:1407:PHE:CZ   | 2.08                     | 1.36              |
| 10:C24:1708:ARG:HH22 | 21:H24:275:LYS:CG    | 1.36                     | 1.36              |
| 10:C24:1708:ARG:NH2  | 21:H24:275:LYS:HG2   | 1.30                     | 1.36              |
| 22:I:131:ARG:HG3     | 23:J32:557:ARG:NH2   | 1.05                     | 1.36              |
| 1:R:768:LEU:CG       | 24:D:1362:VAL:O      | 1.71                     | 1.36              |
| 2:M:428:SER:CB       | 8:L:355:SER:OG       | 1.74                     | 1.36              |
| 12:A:362:ARG:HD2     | 12:A:366:ARG:NH2     | 1.40                     | 1.36              |
| 11:A16:91:GLU:HB2    | 18:B:1112:LYS:NZ     | 1.28                     | 1.36              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A16:445:ASN:HB3   | 17:F8:65:ARG:NH1    | 1.07                     | 1.36              |
| 9:K:743:ARG:NH1      | 9:K:772:TYR:CE1     | 1.94                     | 1.35              |
| 9:K:1232:LEU:CD2     | 9:K:1265:ILE:HG22   | 1.56                     | 1.35              |
| 10:C24:667:ILE:CD1   | 10:C24:697:HIS:HE1  | 1.37                     | 1.35              |
| 13:V:902:MET:CE      | 14:W:777:LEU:HD23   | 1.54                     | 1.35              |
| 11:A32:519:MET:HE1   | 11:A32:569:MET:CE   | 1.56                     | 1.35              |
| 20:E8:434:TRP:NE1    | 24:D40:72:GLU:HB3   | 1.04                     | 1.35              |
| 23:J16:686:MET:HE1   | 23:J16:694:ARG:CZ   | 1.52                     | 1.35              |
| 2:M8:626:PRO:HD2     | 3:N8:165:GLY:O      | 1.22                     | 1.35              |
| 8:L8:1096:GLU:OE1    | 9:K8:996:MET:HB3    | 1.26                     | 1.35              |
| 8:L16:976:LEU:CD2    | 9:K16:1004:ARG:HD3  | 1.55                     | 1.35              |
| 11:A16:519:MET:HE1   | 11:A16:569:MET:CE   | 1.56                     | 1.35              |
| 22:I8:131:ARG:HG3    | 23:J8:557:ARG:NH2   | 1.05                     | 1.35              |
| 24:D:400:VAL:HG11    | 24:D16:751:MET:CB   | 1.54                     | 1.35              |
| 1:R8:983:ARG:O       | 24:D40:1360:ALA:CB  | 1.72                     | 1.35              |
| 10:C16:1074:LEU:HD11 | 10:C16:1075:ASP:OD1 | 1.23                     | 1.35              |
| 18:B8:1439:LYS:HE2   | 24:D32:1257:ASN:CB  | 1.54                     | 1.35              |
| 12:A:519:MET:HE1     | 12:A:569:MET:CE     | 1.56                     | 1.35              |
| 10:C16:1663:SER:CA   | 10:C24:1564:ASP:OD2 | 1.72                     | 1.35              |
| 10:C24:1265:ARG:O    | 10:C24:1268:ARG:CG  | 1.75                     | 1.35              |
| 20:E8:261:PRO:HD2    | 20:E8:305:GLU:OE1   | 1.23                     | 1.35              |
| 24:D:405:GLN:HG2     | 24:D16:10:ARG:CZ    | 1.49                     | 1.35              |
| 9:K:635:ALA:CB       | 9:K:655:GLN:HE22    | 1.39                     | 1.34              |
| 10:C8:898:GLN:NE2    | 10:C8:1138:GLU:OE2  | 1.57                     | 1.34              |
| 11:A16:90:PHE:CG     | 18:B:1788:ILE:CG2   | 2.10                     | 1.34              |
| 2:M16:417:ARG:CD     | 8:L16:298:PHE:HD2   | 1.38                     | 1.34              |
| 5:P16:101:LEU:HD21   | 5:P16:133:TYR:CE1   | 1.59                     | 1.34              |
| 9:K16:894:LYS:NZ     | 9:K16:1057:GLU:HB3  | 1.42                     | 1.34              |
| 10:C16:1265:ARG:O    | 10:C16:1268:ARG:CG  | 1.75                     | 1.34              |
| 10:C8:960:PHE:CZ     | 10:C8:1138:GLU:CD   | 2.06                     | 1.34              |
| 10:C8:960:PHE:CE2    | 10:C8:1138:GLU:HG2  | 1.62                     | 1.34              |
| 18:B:786:ASP:OD2     | 24:D16:1066:VAL:CG2 | 1.72                     | 1.34              |
| 5:P16:101:LEU:CD2    | 5:P16:133:TYR:OH    | 1.69                     | 1.34              |
| 9:K8:1232:LEU:CD2    | 9:K8:1265:ILE:HG22  | 1.56                     | 1.34              |
| 10:C16:407:LYS:HE3   | 10:C16:465:PHE:CE2  | 1.62                     | 1.34              |
| 10:C:667:ILE:CD1     | 10:C:697:HIS:HE1    | 1.37                     | 1.34              |
| 20:E8:432:ILE:HG21   | 24:D40:72:GLU:CD    | 1.48                     | 1.34              |
| 10:C32:1265:ARG:O    | 10:C32:1268:ARG:CG  | 1.75                     | 1.34              |
| 2:M:626:PRO:HD2      | 3:N:165:GLY:O       | 1.22                     | 1.34              |
| 7:Q:341:GLN:HG2      | 10:C8:751:ARG:NH1   | 1.03                     | 1.34              |
| 11:A24:519:MET:HE1   | 11:A24:569:MET:CE   | 1.56                     | 1.34              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:349:PHE:CZ      | 18:B:353:ILE:HD11    | 1.62                     | 1.34              |
| 18:B8:1529:GLU:OE2   | 24:D32:1415:LEU:CD1  | 1.74                     | 1.34              |
| 10:C16:110:ARG:NH1   | 10:C16:118:LEU:HD11  | 1.38                     | 1.34              |
| 10:C16:667:ILE:CD1   | 10:C16:697:HIS:HE1   | 1.36                     | 1.34              |
| 10:C24:1708:ARG:CZ   | 21:H24:279:GLU:OE1   | 1.74                     | 1.34              |
| 18:B8:1575:GLN:NE2   | 24:D32:1403:LEU:HD23 | 1.40                     | 1.34              |
| 1:R:983:ARG:NH2      | 24:D:1366:PRO:HD3    | 1.39                     | 1.33              |
| 10:C16:390:HIS:NE2   | 10:C16:449:GLU:HB3   | 1.05                     | 1.33              |
| 10:C16:390:HIS:NE2   | 10:C16:449:GLU:CB    | 1.88                     | 1.33              |
| 11:A32:445:ASN:HB3   | 17:F24:65:ARG:NH1    | 1.07                     | 1.33              |
| 18:B8:712:PRO:CG     | 18:B8:759:MET:HE1    | 1.55                     | 1.33              |
| 22:I8:131:ARG:CG     | 23:J8:557:ARG:NH2    | 1.90                     | 1.33              |
| 11:A40:519:MET:HE1   | 11:A40:569:MET:CE    | 1.56                     | 1.33              |
| 10:C8:1265:ARG:O     | 10:C8:1268:ARG:CG    | 1.75                     | 1.33              |
| 11:A16:362:ARG:HD2   | 11:A16:366:ARG:NH2   | 1.40                     | 1.33              |
| 18:B8:349:PHE:CZ     | 18:B8:353:ILE:HD11   | 1.62                     | 1.33              |
| 23:J32:686:MET:HE1   | 23:J32:694:ARG:NH2   | 1.39                     | 1.33              |
| 10:C32:110:ARG:NH1   | 10:C32:118:LEU:HD11  | 1.37                     | 1.33              |
| 12:A48:519:MET:HE1   | 12:A48:569:MET:CE    | 1.56                     | 1.33              |
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:CD1    | 1.77                     | 1.33              |
| 10:C:407:LYS:HE3     | 10:C:465:PHE:CZ      | 1.60                     | 1.33              |
| 11:A32:326:TYR:CD1   | 17:F24:77:TYR:HB2    | 1.64                     | 1.33              |
| 18:B:1110:LEU:HD22   | 21:H:326:GLY:N       | 1.43                     | 1.33              |
| 23:J16:686:MET:HE1   | 23:J16:694:ARG:NH2   | 1.39                     | 1.33              |
| 10:C32:407:LYS:CD    | 10:C32:465:PHE:CZ    | 2.11                     | 1.33              |
| 1:R:1121:ARG:C       | 1:R:1122:HIS:N       | 1.87                     | 1.33              |
| 5:P16:101:LEU:HD21   | 5:P16:133:TYR:CZ     | 1.51                     | 1.33              |
| 10:C16:1074:LEU:HD12 | 10:C16:1075:ASP:CA   | 1.57                     | 1.33              |
| 10:C:1265:ARG:O      | 10:C:1268:ARG:CG     | 1.75                     | 1.33              |
| 11:A16:326:TYR:CD1   | 17:F8:77:TYR:HB2     | 1.64                     | 1.33              |
| 18:B8:686:LEU:HD13   | 18:B8:790:ASP:OD2    | 1.25                     | 1.33              |
| 22:I24:131:ARG:CG    | 23:J24:557:ARG:NH2   | 1.90                     | 1.33              |
| 23:J24:686:MET:HE1   | 23:J24:694:ARG:NH2   | 1.39                     | 1.33              |
| 10:C32:407:LYS:HE3   | 10:C32:465:PHE:CE2   | 1.62                     | 1.33              |
| 1:R8:1121:ARG:C      | 1:R8:1122:HIS:N      | 1.87                     | 1.33              |
| 1:R16:1121:ARG:C     | 1:R16:1122:HIS:N     | 1.87                     | 1.33              |
| 5:P8:614:VAL:HB      | 5:P8:629:ARG:NH1     | 1.40                     | 1.33              |
| 8:L16:1068:PHE:HB2   | 9:K16:1285:GLU:OXT   | 1.29                     | 1.33              |
| 9:K8:743:ARG:NH1     | 9:K8:772:TYR:CE1     | 1.94                     | 1.33              |
| 22:I16:131:ARG:CG    | 23:J16:557:ARG:NH2   | 1.90                     | 1.33              |
| 10:C32:1348:LEU:CD1  | 10:C32:1359:ILE:CD1  | 2.07                     | 1.33              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:Q8:124:PHE:CD1    | 7:Q8:125:TYR:CE2    | 2.17                     | 1.32              |
| 19:4:153:ARG:NH2    | 20:E:467:ILE:HD11   | 1.44                     | 1.32              |
| 22:I16:131:ARG:HG3  | 23:J16:557:ARG:NH2  | 1.05                     | 1.32              |
| 5:P:16:PHE:CE1      | 6:O:311:LEU:HD11    | 1.62                     | 1.32              |
| 5:P:600:PHE:CE2     | 5:P:638:SER:OG      | 1.72                     | 1.32              |
| 5:P:607:PHE:CE1     | 5:P:633:LEU:CD1     | 2.09                     | 1.32              |
| 10:C16:1548:ILE:CD1 | 24:D8:1407:PHE:HZ   | 1.23                     | 1.32              |
| 10:C24:110:ARG:NH1  | 10:C24:118:LEU:HD11 | 1.37                     | 1.32              |
| 10:C24:407:LYS:HE3  | 10:C24:465:PHE:CE2  | 1.62                     | 1.32              |
| 22:I:131:ARG:CG     | 23:J32:557:ARG:NH2  | 1.90                     | 1.32              |
| 7:Q:124:PHE:CD1     | 7:Q:125:TYR:CE2     | 2.17                     | 1.32              |
| 11:A24:803:PRO:HB3  | 24:D8:1401:LEU:CD1  | 1.59                     | 1.32              |
| 10:C:1010:ALA:N     | 10:C:1192:ARG:NH2   | 1.78                     | 1.32              |
| 11:A32:91:GLU:HB3   | 18:B8:1112:LYS:CE   | 1.59                     | 1.32              |
| 19:48:342:GLU:OE1   | 24:D8:174:SER:HB3   | 1.16                     | 1.32              |
| 5:P16:16:PHE:CE1    | 6:O16:311:LEU:HD11  | 1.62                     | 1.32              |
| 12:A:642:GLY:CA     | 12:A:685:ARG:CZ     | 2.07                     | 1.32              |
| 22:I24:131:ARG:HG3  | 23:J24:557:ARG:NH2  | 1.05                     | 1.32              |
| 12:A48:362:ARG:HD2  | 12:A48:366:ARG:NH2  | 1.40                     | 1.32              |
| 1:R:1428:VAL:CG2    | 6:O:165:LYS:CE      | 2.07                     | 1.32              |
| 2:M8:669:ALA:HB1    | 2:M8:684:GLN:CG     | 1.46                     | 1.32              |
| 5:P:402:LEU:CD1     | 5:P:433:LEU:HB3     | 1.60                     | 1.32              |
| 10:C24:1272:GLN:OE1 | 10:C24:1289:LYS:CD  | 1.78                     | 1.32              |
| 13:V:790:GLN:NE2    | 14:W:674:GLN:NE2    | 1.72                     | 1.32              |
| 14:W:711:ARG:NH1    | 10:C8:1606:GLY:O    | 1.63                     | 1.32              |
| 18:B:1112:LYS:HE3   | 21:H:327:SER:C      | 1.52                     | 1.32              |
| 18:B8:1110:LEU:HD22 | 21:H24:326:GLY:N    | 1.41                     | 1.32              |
| 20:E8:432:ILE:HD13  | 24:D40:72:GLU:CG    | 1.60                     | 1.32              |
| 10:C32:1010:ALA:N   | 10:C32:1192:ARG:NH2 | 1.77                     | 1.32              |
| 9:K8:578:THR:HG23   | 9:K8:616:ARG:NH2    | 1.37                     | 1.31              |
| 7:Q16:124:PHE:CD1   | 7:Q16:125:TYR:CE2   | 2.17                     | 1.31              |
| 8:L:1081:MET:SD     | 9:K:1083:ILE:CG2    | 2.19                     | 1.31              |
| 9:K8:578:THR:CG2    | 9:K8:616:ARG:HH22   | 1.41                     | 1.31              |
| 10:C:1272:GLN:OE1   | 10:C:1289:LYS:CD    | 1.78                     | 1.31              |
| 10:C:1348:LEU:CD1   | 10:C:1359:ILE:CD1   | 2.07                     | 1.31              |
| 10:C8:668:ALA:C     | 10:C8:669:GLY:N     | 1.83                     | 1.31              |
| 19:48:153:ARG:NH2   | 20:E8:467:ILE:HD11  | 1.44                     | 1.31              |
| 2:M8:428:SER:HB2    | 8:L8:355:SER:OG     | 1.18                     | 1.31              |
| 5:P16:112:LEU:CD2   | 5:P16:122:TYR:CD1   | 1.87                     | 1.31              |
| 10:C16:1285:VAL:CG2 | 10:C16:1738:MET:CE  | 1.88                     | 1.31              |
| 10:C24:1285:VAL:CG2 | 10:C24:1738:MET:CE  | 1.88                     | 1.31              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 20:E8:432:ILE:CD1   | 24:D40:72:GLU:CG     | 2.08                     | 1.31              |
| 20:E8:434:TRP:HE1   | 24:D40:72:GLU:CG     | 1.43                     | 1.31              |
| 10:C16:407:LYS:CD   | 10:C16:465:PHE:CZ    | 2.11                     | 1.31              |
| 11:A40:468:VAL:CG2  | 24:D32:1103:LEU:HD12 | 1.60                     | 1.31              |
| 18:B:786:ASP:CG     | 24:D16:1066:VAL:HG22 | 1.41                     | 1.31              |
| 10:C32:1272:GLN:OE1 | 10:C32:1289:LYS:CD   | 1.78                     | 1.31              |
| 5:P8:16:PHE:CE1     | 6:O8:311:LEU:HD11    | 1.62                     | 1.31              |
| 10:C16:1272:GLN:OE1 | 10:C16:1289:LYS:CD   | 1.77                     | 1.31              |
| 11:A24:326:TYR:CD1  | 17:F:77:TYR:HB2      | 1.64                     | 1.31              |
| 10:C24:407:LYS:CD   | 10:C24:465:PHE:CZ    | 2.11                     | 1.31              |
| 10:C8:1272:GLN:OE1  | 10:C8:1289:LYS:CD    | 1.78                     | 1.31              |
| 8:L16:177:ARG:CD    | 12:A48:744:GLU:OE1   | 1.78                     | 1.30              |
| 10:C24:1348:LEU:CD1 | 10:C24:1359:ILE:CD1  | 2.07                     | 1.30              |
| 11:A40:326:TYR:CD1  | 17:F16:77:TYR:HB2    | 1.64                     | 1.30              |
| 11:A40:474:LEU:HD13 | 24:D32:1099:ARG:CZ   | 1.61                     | 1.30              |
| 10:C:979:MET:CE     | 10:C:1028:ILE:CG2    | 2.08                     | 1.30              |
| 1:R:983:ARG:O       | 24:D:1360:ALA:CB     | 1.75                     | 1.30              |
| 9:K:792:LEU:CD1     | 9:K:864:ILE:HD11     | 1.59                     | 1.30              |
| 10:C16:1348:LEU:CD1 | 10:C16:1359:ILE:CD1  | 2.07                     | 1.30              |
| 10:C:1285:VAL:CG2   | 10:C:1738:MET:CE     | 1.88                     | 1.30              |
| 2:M16:626:PRO:HD2   | 3:N16:165:GLY:O      | 1.22                     | 1.30              |
| 7:Q:297:VAL:CG1     | 7:Q:301:ARG:HB2      | 1.61                     | 1.30              |
| 9:K:578:THR:HG23    | 9:K:616:ARG:NH2      | 1.37                     | 1.30              |
| 9:K:649:MET:HB3     | 9:K:704:ARG:NH2      | 1.46                     | 1.30              |
| 11:A32:445:ASN:CB   | 17:F24:65:ARG:HH12   | 1.43                     | 1.30              |
| 23:J8:686:MET:HE1   | 23:J8:694:ARG:NH2    | 1.39                     | 1.30              |
| 2:M8:785:ASP:N      | 8:L16:472:GLU:OE2    | 1.61                     | 1.30              |
| 7:Q8:297:VAL:CG1    | 7:Q8:301:ARG:HB2     | 1.61                     | 1.30              |
| 10:C16:1699:LYS:NZ  | 23:J32:722:LEU:HD22  | 1.45                     | 1.30              |
| 10:C8:1348:LEU:CD1  | 10:C8:1359:ILE:CD1   | 2.07                     | 1.30              |
| 11:A32:362:ARG:HD2  | 11:A32:366:ARG:NH2   | 1.40                     | 1.30              |
| 20:E:344:PRO:HA     | 24:D:121:GLU:OE2     | 1.17                     | 1.30              |
| 10:C24:1814:LYS:NZ  | 23:J24:738:MET:CB    | 1.95                     | 1.30              |
| 18:B:1112:LYS:HE3   | 21:H:327:SER:CA      | 1.61                     | 1.30              |
| 18:B:1529:GLU:OE2   | 24:D16:1415:LEU:HD11 | 1.14                     | 1.30              |
| 22:I24:196:VAL:CA   | 23:J24:620:MET:HE1   | 1.62                     | 1.30              |
| 9:K:578:THR:CG2     | 9:K:616:ARG:HH22     | 1.41                     | 1.29              |
| 15:J:623:GLU:OE2    | 15:J:626:ARG:NH2     | 1.62                     | 1.29              |
| 11:A16:707:LEU:HB2  | 24:D16:1398:ARG:NH2  | 1.47                     | 1.29              |
| 22:I:196:VAL:CA     | 23:J32:620:MET:HE1   | 1.62                     | 1.29              |
| 2:M8:417:ARG:NH2    | 8:L8:415:PHE:CE2     | 2.00                     | 1.29              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M8:672:TYR:CB     | 2:M8:680:LYS:CD      | 1.83                     | 1.29              |
| 10:C16:1010:ALA:N   | 10:C16:1192:ARG:NH2  | 1.77                     | 1.29              |
| 10:C16:1814:LYS:NZ  | 23:J32:738:MET:HB3   | 1.46                     | 1.29              |
| 10:C:407:LYS:CE     | 10:C:465:PHE:CZ      | 2.14                     | 1.29              |
| 10:C:679:ARG:NH2    | 10:C:690:LEU:HD21    | 1.47                     | 1.29              |
| 2:M8:672:TYR:CB     | 2:M8:680:LYS:HD2     | 1.50                     | 1.29              |
| 7:Q8:124:PHE:HE1    | 7:Q8:125:TYR:OH      | 1.16                     | 1.29              |
| 10:C16:390:HIS:CD2  | 10:C16:452:LEU:CB    | 2.13                     | 1.29              |
| 11:A24:787:ASP:O    | 11:A24:836:LYS:NZ    | 1.66                     | 1.29              |
| 10:C24:668:ALA:C    | 10:C24:669:GLY:N     | 1.83                     | 1.29              |
| 20:E:261:PRO:HD2    | 20:E:305:GLU:OE1     | 1.22                     | 1.29              |
| 24:D32:642:VAL:HG22 | 24:D40:631:ARG:CZ    | 1.60                     | 1.29              |
| 10:C24:1010:ALA:N   | 10:C24:1192:ARG:NH2  | 1.77                     | 1.29              |
| 10:C:35:ASN:OD1     | 24:D:1148:LEU:HD12   | 1.24                     | 1.29              |
| 11:A16:787:ASP:O    | 11:A16:836:LYS:NZ    | 1.66                     | 1.29              |
| 18:B8:1618:HIS:CE1  | 18:B8:1622:ILE:HD11  | 1.68                     | 1.29              |
| 10:C8:1010:ALA:N    | 10:C8:1192:ARG:NH2   | 1.77                     | 1.29              |
| 10:C32:1318:ARG:NH2 | 10:C32:1396:SER:OG   | 1.66                     | 1.29              |
| 12:A48:787:ASP:O    | 12:A48:836:LYS:NZ    | 1.66                     | 1.29              |
| 7:Q16:297:VAL:CG1   | 7:Q16:301:ARG:HB2    | 1.61                     | 1.28              |
| 18:B:1102:LYS:NZ    | 18:B:1354:ASP:OD2    | 1.63                     | 1.28              |
| 24:D40:839:GLU:OE2  | 24:D40:971:HIS:CB    | 1.79                     | 1.28              |
| 2:M:672:TYR:CD1     | 2:M:680:LYS:NZ       | 2.01                     | 1.28              |
| 10:C16:1251:PHE:CZ  | 10:C16:1319:ARG:NH1  | 2.02                     | 1.28              |
| 10:C:407:LYS:CE     | 10:C:465:PHE:HZ      | 1.46                     | 1.28              |
| 18:B:1618:HIS:CE1   | 18:B:1622:ILE:HD11   | 1.68                     | 1.28              |
| 18:B:1673:ARG:O     | 18:B:1676:VAL:HG23   | 1.31                     | 1.28              |
| 1:R:1324:ASP:CG     | 10:C:1180:ILE:HG21   | 1.58                     | 1.28              |
| 5:P:401:ARG:CG      | 5:P:414:VAL:HG11     | 1.62                     | 1.28              |
| 8:L8:976:LEU:HD23   | 9:K8:1004:ARG:NE     | 1.48                     | 1.28              |
| 11:A40:474:LEU:CD1  | 24:D32:1099:ARG:HH22 | 1.47                     | 1.28              |
| 11:A40:787:ASP:O    | 11:A40:836:LYS:NZ    | 1.66                     | 1.28              |
| 10:C:153:ALA:HB1    | 24:D:1403:LEU:CG     | 1.62                     | 1.28              |
| 18:B8:1439:LYS:NZ   | 24:D32:1257:ASN:HB3  | 1.45                     | 1.28              |
| 4:T16:674:GLN:OE1   | 5:P16:695:GLN:NE2    | 1.63                     | 1.28              |
| 9:K:1154:TRP:CZ2    | 9:K:1219:VAL:HG11    | 1.68                     | 1.28              |
| 9:K8:635:ALA:CA     | 9:K8:655:GLN:HE22    | 1.44                     | 1.28              |
| 11:A32:91:GLU:CB    | 18:B8:1112:LYS:HZ3   | 1.40                     | 1.28              |
| 18:B8:1210:CYS:SG   | 18:B8:1234:MET:CE    | 2.19                     | 1.28              |
| 22:I8:196:VAL:CA    | 23:J8:620:MET:HE1    | 1.62                     | 1.28              |
| 10:C:1251:PHE:CZ    | 10:C:1319:ARG:NH1    | 2.02                     | 1.28              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:690:TRP:CE3    | 18:B:739:VAL:HG21   | 1.67                     | 1.28              |
| 3:N16:4:GLN:HE22    | 3:N16:44:GLY:CA     | 1.46                     | 1.27              |
| 10:C16:668:ALA:C    | 10:C16:669:GLY:N    | 1.83                     | 1.27              |
| 10:C16:1318:ARG:NH2 | 10:C16:1396:SER:OG  | 1.66                     | 1.27              |
| 10:C16:1547:LYS:HD3 | 24:D8:1406:SER:N    | 1.48                     | 1.27              |
| 10:C24:1251:PHE:CZ  | 10:C24:1319:ARG:NH1 | 2.02                     | 1.27              |
| 14:W:584:CYS:SG     | 15:J:573:LYS:CE     | 2.22                     | 1.27              |
| 20:E8:123:CYS:SG    | 20:E8:135:ILE:CD1   | 2.22                     | 1.27              |
| 18:B:421:ASP:OD1    | 18:B:468:ARG:NH2    | 1.66                     | 1.27              |
| 18:B8:421:ASP:OD1   | 18:B8:468:ARG:NH2   | 1.65                     | 1.27              |
| 18:B8:690:TRP:CE3   | 18:B8:739:VAL:HG21  | 1.67                     | 1.27              |
| 2:M16:816:ARG:HH12  | 2:M16:849:LEU:CB    | 1.47                     | 1.27              |
| 10:C8:572:ILE:CD1   | 10:C8:606:MET:HE2   | 1.65                     | 1.27              |
| 10:C8:1318:ARG:NH2  | 10:C8:1396:SER:OG   | 1.67                     | 1.27              |
| 18:B:1210:CYS:SG    | 18:B:1234:MET:CE    | 2.19                     | 1.27              |
| 18:B8:1102:LYS:NZ   | 18:B8:1354:ASP:OD2  | 1.63                     | 1.27              |
| 20:E:123:CYS:SG     | 20:E:135:ILE:CD1    | 2.22                     | 1.27              |
| 3:N:4:GLN:HE22      | 3:N:44:GLY:CA       | 1.46                     | 1.27              |
| 1:R8:1185:THR:HG21  | 24:D40:1462:PHE:CZ  | 1.70                     | 1.27              |
| 2:M8:202:LYS:NZ     | 2:M8:208:SER:O      | 1.65                     | 1.27              |
| 5:P:401:ARG:HD2     | 5:P:414:VAL:CG2     | 1.62                     | 1.27              |
| 9:K:635:ALA:CA      | 9:K:655:GLN:HE22    | 1.44                     | 1.27              |
| 10:C8:1251:PHE:CZ   | 10:C8:1319:ARG:NH1  | 2.02                     | 1.27              |
| 18:B8:1673:ARG:O    | 18:B8:1676:VAL:HG23 | 1.30                     | 1.27              |
| 22:I:146:SER:CB     | 23:J32:574:ARG:HH12 | 1.47                     | 1.27              |
| 24:D:405:GLN:CG     | 24:D16:10:ARG:CZ    | 2.08                     | 1.27              |
| 2:M:202:LYS:NZ      | 2:M:208:SER:O       | 1.65                     | 1.27              |
| 2:M16:202:LYS:NZ    | 2:M16:208:SER:O     | 1.65                     | 1.27              |
| 2:M16:628:LEU:HD13  | 3:N16:223:GLY:O     | 1.35                     | 1.27              |
| 6:O8:179:LYS:HD3    | 6:O8:183:GLN:CD     | 1.59                     | 1.27              |
| 10:C24:1545:ARG:NH2 | 11:A40:672:GLU:OE2  | 1.67                     | 1.27              |
| 10:C:668:ALA:C      | 10:C:669:GLY:N      | 1.83                     | 1.27              |
| 18:B:140:GLN:NE2    | 18:B:206:GLU:OE2    | 1.68                     | 1.27              |
| 18:B8:1110:LEU:CD2  | 21:H24:326:GLY:H    | 1.47                     | 1.27              |
| 20:E:123:CYS:SG     | 20:E:135:ILE:HD13   | 1.74                     | 1.27              |
| 19:48:365:GLU:OE2   | 19:48:442:ARG:NH2   | 1.67                     | 1.27              |
| 22:I16:146:SER:CB   | 23:J16:574:ARG:HH12 | 1.47                     | 1.27              |
| 22:I16:196:VAL:CA   | 23:J16:620:MET:HE1  | 1.62                     | 1.27              |
| 24:D:405:GLN:HG2    | 24:D16:10:ARG:NH1   | 0.95                     | 1.27              |
| 2:M8:351:ALA:CB     | 8:L8:219:ILE:CG2    | 2.13                     | 1.26              |
| 3:N8:4:GLN:HE22     | 3:N8:44:GLY:CA      | 1.46                     | 1.26              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A32:787:ASP:O    | 11:A32:836:LYS:NZ   | 1.66                     | 1.26              |
| 18:B:751:TYR:OH     | 18:B:804:ARG:NH1    | 1.68                     | 1.26              |
| 20:E:344:PRO:HA     | 24:D:121:GLU:CD     | 1.58                     | 1.26              |
| 2:M16:639:GLN:NE2   | 3:N16:269:LEU:HD13  | 1.50                     | 1.26              |
| 9:K8:1154:TRP:CZ2   | 9:K8:1219:VAL:HG11  | 1.68                     | 1.26              |
| 10:C24:1548:ILE:CD1 | 24:D24:1407:PHE:CE2 | 2.17                     | 1.26              |
| 14:W:516:GLN:HA     | 14:W:604:PRO:C      | 1.60                     | 1.26              |
| 10:C:1318:ARG:NH2   | 10:C:1396:SER:OG    | 1.67                     | 1.26              |
| 18:B8:1529:GLU:OE2  | 24:D32:1415:LEU:CG  | 1.83                     | 1.26              |
| 22:I24:146:SER:CB   | 23:J24:574:ARG:HH12 | 1.47                     | 1.26              |
| 10:C32:390:HIS:ND1  | 10:C32:452:LEU:HD13 | 1.50                     | 1.26              |
| 10:C32:1251:PHE:CZ  | 10:C32:1319:ARG:NH1 | 2.02                     | 1.26              |
| 5:P16:527:LYS:HE3   | 6:O16:68:GLU:OE1    | 1.08                     | 1.26              |
| 11:A24:445:ASN:CB   | 17:F:65:ARG:HH12    | 1.43                     | 1.26              |
| 11:A24:645:GLU:HG2  | 24:D16:867:ASP:OD1  | 1.09                     | 1.26              |
| 1:R:1290:ILE:CD1    | 10:C:605:GLU:OE2    | 1.82                     | 1.26              |
| 2:M16:231:ARG:HD2   | 2:M16:299:GLY:CA    | 1.63                     | 1.26              |
| 5:P8:527:LYS:HE3    | 6:O8:68:GLU:OE1     | 1.08                     | 1.26              |
| 7:Q16:124:PHE:HE1   | 7:Q16:125:TYR:OH    | 1.16                     | 1.26              |
| 11:A40:445:ASN:CB   | 17:F16:65:ARG:HH12  | 1.43                     | 1.26              |
| 14:W:631:TYR:CZ     | 15:J:554:LEU:HD21   | 1.69                     | 1.26              |
| 18:B8:751:TYR:OH    | 18:B8:804:ARG:NH1   | 1.68                     | 1.26              |
| 10:C32:572:ILE:CD1  | 10:C32:606:MET:HE2  | 1.65                     | 1.26              |
| 2:M:844:VAL:CG2     | 4:T:660:LEU:CD2     | 2.14                     | 1.26              |
| 1:R8:1466:LYS:HB3   | 6:O8:160:LEU:CD1    | 1.63                     | 1.26              |
| 5:P:527:LYS:HE3     | 6:O:68:GLU:OE1      | 1.08                     | 1.26              |
| 12:A:787:ASP:O      | 12:A:836:LYS:NZ     | 1.66                     | 1.26              |
| 10:C:572:ILE:CD1    | 10:C:606:MET:HE2    | 1.65                     | 1.26              |
| 11:A16:90:PHE:CD2   | 18:B:1788:ILE:CG2   | 2.17                     | 1.26              |
| 1:R8:982:GLU:OE1    | 24:D40:1436:ARG:HB3 | 1.28                     | 1.25              |
| 2:M16:417:ARG:HB3   | 8:L16:298:PHE:CE2   | 1.68                     | 1.25              |
| 5:P8:610:SER:O      | 5:P8:629:ARG:NH2    | 1.68                     | 1.25              |
| 9:K:840:TRP:CZ3     | 9:K:907:ILE:HD11    | 1.70                     | 1.25              |
| 9:K8:649:MET:HB3    | 9:K8:704:ARG:NH2    | 1.46                     | 1.25              |
| 11:A32:629:LEU:O    | 11:A32:678:LYS:NZ   | 1.69                     | 1.25              |
| 2:M:816:ARG:HH12    | 2:M:849:LEU:CB      | 1.47                     | 1.25              |
| 1:R8:768:LEU:HG     | 24:D40:1362:VAL:O   | 1.30                     | 1.25              |
| 5:P:322:CYS:HB2     | 13:V:767:GLU:OE1    | 1.35                     | 1.25              |
| 9:K:792:LEU:CD1     | 9:K:864:ILE:HD13    | 1.60                     | 1.25              |
| 10:C16:572:ILE:CD1  | 10:C16:606:MET:HE2  | 1.65                     | 1.25              |
| 14:W:515:CYS:CB     | 14:W:604:PRO:CD     | 2.01                     | 1.25              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:1166:SER:O     | 10:C:1168:PRO:CD     | 1.84                     | 1.25              |
| 11:A32:212:LYS:HE3  | 11:A32:585:MET:CE    | 1.63                     | 1.25              |
| 18:B8:786:ASP:OD1   | 24:D32:1066:VAL:HG13 | 1.18                     | 1.25              |
| 1:R:1290:ILE:HD11   | 10:C:605:GLU:OE2     | 1.09                     | 1.25              |
| 3:N8:19:MET:HE2     | 3:N8:23:GLY:C        | 1.62                     | 1.25              |
| 2:M16:844:VAL:CG2   | 4:T16:660:LEU:CD2    | 2.13                     | 1.25              |
| 5:P:179:TYR:CE1     | 5:P:437:GLY:HA3      | 1.69                     | 1.25              |
| 8:L16:1096:GLU:OE2  | 9:K16:998:GLN:HG2    | 1.16                     | 1.25              |
| 10:C24:1699:LYS:NZ  | 23:J24:722:LEU:CD2   | 1.98                     | 1.25              |
| 21:H8:312:GLN:CG    | 21:H8:316:ILE:HD11   | 1.67                     | 1.25              |
| 12:A48:212:LYS:HE3  | 12:A48:585:MET:CE    | 1.63                     | 1.25              |
| 12:A:707:LEU:CG     | 12:A:767:ARG:HH22    | 1.50                     | 1.25              |
| 18:B8:140:GLN:NE2   | 18:B8:206:GLU:OE2    | 1.68                     | 1.25              |
| 1:R8:1266:THR:CA    | 5:P8:684:ARG:NH2     | 1.98                     | 1.25              |
| 6:O:179:LYS:HD3     | 6:O:183:GLN:CD       | 1.60                     | 1.25              |
| 6:O16:179:LYS:HD3   | 6:O16:183:GLN:CD     | 1.59                     | 1.25              |
| 8:L16:976:LEU:HD21  | 9:K16:1004:ARG:CD    | 1.67                     | 1.25              |
| 10:C24:572:ILE:HD11 | 10:C24:606:MET:CE    | 1.67                     | 1.25              |
| 10:C24:1318:ARG:NH2 | 10:C24:1396:SER:OG   | 1.66                     | 1.25              |
| 10:C8:1166:SER:O    | 10:C8:1168:PRO:CD    | 1.84                     | 1.25              |
| 19:4:183:ARG:HH12   | 19:4:245:GLY:CA      | 1.50                     | 1.25              |
| 20:E8:123:CYS:SG    | 20:E8:135:ILE:HD13   | 1.74                     | 1.25              |
| 10:C32:572:ILE:HD11 | 10:C32:606:MET:CE    | 1.67                     | 1.25              |
| 2:M:639:GLN:NE2     | 3:N:269:LEU:HD13     | 1.50                     | 1.25              |
| 2:M8:816:ARG:HH12   | 2:M8:849:LEU:CB      | 1.47                     | 1.25              |
| 10:C16:572:ILE:HD11 | 10:C16:606:MET:CE    | 1.67                     | 1.25              |
| 14:W:590:LEU:CD1    | 14:W:641:GLU:OE2     | 1.85                     | 1.25              |
| 11:A16:91:GLU:OE2   | 18:B:1112:LYS:CD     | 1.83                     | 1.25              |
| 18:B:779:LYS:HE3    | 18:B:847:GLN:NE2     | 1.50                     | 1.25              |
| 18:B8:1575:GLN:HE21 | 24:D32:1403:LEU:CD2  | 1.48                     | 1.25              |
| 21:H8:267:LYS:NZ    | 23:J8:631:GLU:OE2    | 1.70                     | 1.25              |
| 10:C32:679:ARG:NH2  | 10:C32:690:LEU:HD21  | 1.48                     | 1.25              |
| 12:A48:806:GLN:CD   | 12:A48:847:ARG:HH22  | 1.45                     | 1.25              |
| 2:M:833:GLU:OE1     | 4:T:667:ILE:HA       | 1.37                     | 1.24              |
| 2:M8:162:ILE:HD11   | 2:M8:213:LEU:CG      | 1.66                     | 1.24              |
| 2:M8:844:VAL:CG2    | 4:T8:660:LEU:CD2     | 2.13                     | 1.24              |
| 2:M16:162:ILE:HD11  | 2:M16:213:LEU:CG     | 1.66                     | 1.24              |
| 9:K8:840:TRP:CZ3    | 9:K8:907:ILE:HD11    | 1.70                     | 1.24              |
| 10:C16:1453:ARG:NH2 | 24:D8:1150:GLY:HA3   | 1.50                     | 1.24              |
| 11:A24:707:LEU:CG   | 11:A24:767:ARG:HH22  | 1.50                     | 1.24              |
| 10:C24:572:ILE:CD1  | 10:C24:606:MET:HE2   | 1.65                     | 1.24              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 11:A40:707:LEU:CG  | 11:A40:767:ARG:HH22  | 1.50                     | 1.24              |
| 11:A32:707:LEU:CG  | 11:A32:767:ARG:HH22  | 1.49                     | 1.24              |
| 12:A48:707:LEU:CG  | 12:A48:767:ARG:HH22  | 1.50                     | 1.24              |
| 6:O8:61:LYS:NZ     | 6:O8:112:ASP:OD1     | 1.69                     | 1.24              |
| 11:A24:212:LYS:HE3 | 11:A24:585:MET:CE    | 1.63                     | 1.24              |
| 12:A:798:PHE:CE1   | 12:A:847:ARG:NH1     | 2.05                     | 1.24              |
| 11:A16:445:ASN:HB3 | 17:F8:65:ARG:CZ      | 1.68                     | 1.24              |
| 11:A16:629:LEU:O   | 11:A16:678:LYS:NZ    | 1.69                     | 1.24              |
| 11:A32:798:PHE:CE1 | 11:A32:847:ARG:NH1   | 2.05                     | 1.24              |
| 19:4:250:ILE:CG2   | 20:E:165:ARG:NH2     | 1.99                     | 1.24              |
| 22:I8:146:SER:CB   | 23:J8:574:ARG:HH12   | 1.47                     | 1.24              |
| 10:C32:1166:SER:O  | 10:C32:1168:PRO:CD   | 1.84                     | 1.24              |
| 12:A48:798:PHE:CE1 | 12:A48:847:ARG:NH1   | 2.05                     | 1.24              |
| 2:M:162:ILE:HD11   | 2:M:213:LEU:CG       | 1.66                     | 1.24              |
| 3:N:1:MET:HB2      | 3:N:302:PRO:C        | 1.61                     | 1.24              |
| 11:A40:445:ASN:HB3 | 17:F16:65:ARG:CZ     | 1.68                     | 1.24              |
| 12:A:642:GLY:HA3   | 12:A:685:ARG:NH2     | 1.52                     | 1.24              |
| 11:A16:798:PHE:CE1 | 11:A16:847:ARG:NH1   | 2.05                     | 1.24              |
| 18:B:846:SER:OG    | 18:B:899:LYS:NZ      | 1.68                     | 1.24              |
| 18:B:1256:THR:CG2  | 24:D16:1238:GLU:HG3  | 1.65                     | 1.24              |
| 10:C32:668:ALA:C   | 10:C32:669:GLY:N     | 1.83                     | 1.24              |
| 3:N:19:MET:HE2     | 3:N:23:GLY:C         | 1.62                     | 1.24              |
| 2:M16:417:ARG:CB   | 8:L16:298:PHE:HE2    | 1.49                     | 1.24              |
| 5:P:15:LEU:CD2     | 6:O:309:SER:O        | 1.84                     | 1.24              |
| 8:L:1096:GLU:OE1   | 9:K:996:MET:O        | 1.54                     | 1.24              |
| 9:K:840:TRP:HZ3    | 9:K:907:ILE:CD1      | 1.50                     | 1.24              |
| 9:K:1232:LEU:HD21  | 9:K:1265:ILE:CG2     | 1.68                     | 1.24              |
| 9:K8:840:TRP:HZ3   | 9:K8:907:ILE:CD1     | 1.50                     | 1.24              |
| 11:A24:35:ARG:NH2  | 22:I8:282:GLU:OE1    | 1.70                     | 1.24              |
| 11:A24:629:LEU:O   | 11:A24:678:LYS:NZ    | 1.69                     | 1.24              |
| 12:A:806:GLN:CD    | 12:A:847:ARG:HH22    | 1.45                     | 1.24              |
| 11:A32:388:VAL:H   | 11:A32:459:ARG:NH1   | 1.36                     | 1.24              |
| 18:B:786:ASP:OD2   | 24:D16:1066:VAL:HG22 | 1.22                     | 1.24              |
| 18:B8:410:GLN:HE21 | 18:B8:538:ARG:NH2    | 1.32                     | 1.24              |
| 24:D:1099:ARG:CZ   | 24:D:1149:VAL:HG21   | 1.68                     | 1.24              |
| 1:R:983:ARG:O      | 24:D:1360:ALA:HB1    | 1.32                     | 1.24              |
| 2:M16:401:ARG:NH2  | 8:L16:381:GLU:HB3    | 1.53                     | 1.24              |
| 9:K8:1232:LEU:HD21 | 9:K8:1265:ILE:CG2    | 1.68                     | 1.24              |
| 18:B:1529:GLU:OE2  | 24:D16:1415:LEU:CG   | 1.85                     | 1.24              |
| 3:N16:1:MET:HB2    | 3:N16:302:PRO:C      | 1.61                     | 1.23              |
| 6:O:61:LYS:NZ      | 6:O:112:ASP:OD1      | 1.69                     | 1.23              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 7:Q:124:PHE:HE1      | 7:Q:125:TYR:OH      | 1.16                     | 1.23              |
| 11:A24:798:PHE:CE1   | 11:A24:847:ARG:NH1  | 2.05                     | 1.23              |
| 10:C:979:MET:CE      | 10:C:1028:ILE:HG22  | 1.63                     | 1.23              |
| 11:A32:445:ASN:HB3   | 17:F24:65:ARG:CZ    | 1.68                     | 1.23              |
| 18:B:410:GLN:HE21    | 18:B:538:ARG:NH2    | 1.32                     | 1.23              |
| 12:A48:629:LEU:O     | 12:A48:678:LYS:NZ   | 1.69                     | 1.23              |
| 2:M8:628:LEU:HD13    | 3:N8:223:GLY:O      | 1.35                     | 1.23              |
| 5:P8:15:LEU:CD2      | 6:O8:309:SER:O      | 1.84                     | 1.23              |
| 5:P16:15:LEU:CD2     | 6:O16:309:SER:O     | 1.85                     | 1.23              |
| 6:O16:61:LYS:NZ      | 6:O16:112:ASP:OD1   | 1.69                     | 1.23              |
| 10:C16:565:ARG:CD    | 10:C16:568:TRP:CE3  | 2.22                     | 1.23              |
| 10:C24:1348:LEU:HD13 | 10:C24:1359:ILE:CD1 | 1.68                     | 1.23              |
| 11:A40:35:ARG:NH2    | 22:I16:282:GLU:OE1  | 1.70                     | 1.23              |
| 10:C:407:LYS:CD      | 10:C:465:PHE:CZ     | 2.21                     | 1.23              |
| 11:A16:806:GLN:CD    | 11:A16:847:ARG:HH22 | 1.45                     | 1.23              |
| 18:B8:779:LYS:HE3    | 18:B8:847:GLN:NE2   | 1.50                     | 1.23              |
| 21:H16:267:LYS:NZ    | 23:J16:631:GLU:OE2  | 1.70                     | 1.23              |
| 24:D:405:GLN:CD      | 24:D16:10:ARG:NE    | 1.71                     | 1.23              |
| 24:D40:839:GLU:OE2   | 24:D40:971:HIS:CG   | 1.92                     | 1.23              |
| 2:M16:627:TYR:CE1    | 3:N16:166:ALA:O     | 1.91                     | 1.23              |
| 8:L16:851:PRO:CG     | 9:K16:1283:PRO:CB   | 1.90                     | 1.23              |
| 10:C24:565:ARG:CD    | 10:C24:568:TRP:CE3  | 2.21                     | 1.23              |
| 11:A40:474:LEU:HD13  | 24:D32:1099:ARG:NH2 | 1.52                     | 1.23              |
| 11:A40:798:PHE:CE1   | 11:A40:847:ARG:NH1  | 2.05                     | 1.23              |
| 11:A16:676:TYR:CE2   | 24:D16:1396:PRO:HD2 | 1.73                     | 1.23              |
| 11:A16:707:LEU:CG    | 11:A16:767:ARG:HH22 | 1.49                     | 1.23              |
| 21:H:312:GLN:CG      | 21:H:316:ILE:HD11   | 1.67                     | 1.23              |
| 21:H8:322:LEU:HB3    | 22:I8:300:LEU:CD1   | 1.69                     | 1.23              |
| 22:I24:131:ARG:HG3   | 23:J24:557:ARG:CZ   | 1.69                     | 1.23              |
| 10:C16:1166:SER:O    | 10:C16:1168:PRO:CD  | 1.84                     | 1.23              |
| 11:A24:806:GLN:CD    | 11:A24:847:ARG:HH22 | 1.45                     | 1.23              |
| 11:A40:388:VAL:H     | 11:A40:459:ARG:NH1  | 1.36                     | 1.23              |
| 11:A40:629:LEU:O     | 11:A40:678:LYS:NZ   | 1.69                     | 1.23              |
| 10:C8:572:ILE:HD11   | 10:C8:606:MET:CE    | 1.67                     | 1.23              |
| 11:A32:806:GLN:CD    | 11:A32:847:ARG:HH22 | 1.45                     | 1.23              |
| 21:H16:312:GLN:CG    | 21:H16:316:ILE:HD11 | 1.67                     | 1.23              |
| 2:M8:639:GLN:NE2     | 3:N8:269:LEU:HD13   | 1.50                     | 1.23              |
| 2:M8:669:ALA:HB2     | 2:M8:684:GLN:NE2    | 1.51                     | 1.23              |
| 2:M16:231:ARG:NE     | 2:M16:299:GLY:CA    | 2.01                     | 1.23              |
| 8:L16:976:LEU:CD2    | 9:K16:1004:ARG:CD   | 2.15                     | 1.23              |
| 9:K:916:LYS:CG       | 9:K:919:MET:HE2     | 1.67                     | 1.23              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A24:803:PRO:CB    | 24:D8:1401:LEU:HD12 | 1.66                     | 1.23              |
| 10:C24:1166:SER:O    | 10:C24:1168:PRO:CD  | 1.84                     | 1.23              |
| 10:C:572:ILE:HD11    | 10:C:606:MET:CE     | 1.67                     | 1.23              |
| 10:C:960:PHE:HZ      | 10:C:1138:GLU:OE2   | 1.22                     | 1.23              |
| 19:48:250:ILE:CG2    | 20:E8:165:ARG:NH2   | 1.99                     | 1.23              |
| 2:M:399:THR:CB       | 2:M:480:ARG:HH21    | 1.52                     | 1.22              |
| 8:L8:605:MET:SD      | 8:L8:631:LEU:HD12   | 1.79                     | 1.22              |
| 10:C24:1272:GLN:OE1  | 10:C24:1289:LYS:HD2 | 1.32                     | 1.22              |
| 14:W:715:ASP:CA      | 10:C8:1568:ARG:NH1  | 2.00                     | 1.22              |
| 21:H:322:LEU:HB3     | 22:I:300:LEU:CD1    | 1.69                     | 1.22              |
| 24:D:409:LEU:HD13    | 24:D16:746:ALA:N    | 1.50                     | 1.22              |
| 2:M8:351:ALA:CB      | 8:L8:219:ILE:HG21   | 1.66                     | 1.22              |
| 5:P:600:PHE:CE2      | 5:P:638:SER:HB2     | 1.69                     | 1.22              |
| 9:K8:1085:TYR:OH     | 9:K8:1093:SER:HA    | 1.05                     | 1.22              |
| 11:A24:445:ASN:CG    | 17:F:65:ARG:HH12    | 1.46                     | 1.22              |
| 18:B8:846:SER:OG     | 18:B8:899:LYS:NZ    | 1.68                     | 1.22              |
| 18:B8:1110:LEU:CD2   | 21:H24:326:GLY:HA2  | 1.70                     | 1.22              |
| 12:A48:388:VAL:H     | 12:A48:459:ARG:NH1  | 1.36                     | 1.22              |
| 1:R:1185:THR:HG21    | 24:D:1462:PHE:CZ    | 1.75                     | 1.22              |
| 3:N8:1:MET:HB2       | 3:N8:302:PRO:C      | 1.61                     | 1.22              |
| 11:A24:445:ASN:HB3   | 17:F:65:ARG:CZ      | 1.68                     | 1.22              |
| 10:C24:1814:LYS:HZ1  | 23:J24:738:MET:CB   | 1.49                     | 1.22              |
| 12:A:388:VAL:H       | 12:A:459:ARG:NH1    | 1.36                     | 1.22              |
| 14:W:516:GLN:CA      | 14:W:604:PRO:O      | 1.88                     | 1.22              |
| 11:A16:445:ASN:CB    | 17:F8:65:ARG:HH12   | 1.43                     | 1.22              |
| 11:A16:676:TYR:OH    | 24:D16:1395:SER:HA  | 1.08                     | 1.22              |
| 11:A16:676:TYR:CE2   | 24:D16:1395:SER:HA  | 1.74                     | 1.22              |
| 19:48:183:ARG:HH12   | 19:48:245:GLY:CA    | 1.50                     | 1.22              |
| 21:H24:322:LEU:HB3   | 22:I24:300:LEU:CD1  | 1.69                     | 1.22              |
| 24:D24:857:THR:HB    | 24:D24:885:TYR:OH   | 1.35                     | 1.22              |
| 3:N16:19:MET:HE2     | 3:N16:23:GLY:C      | 1.62                     | 1.22              |
| 8:L8:605:MET:SD      | 8:L8:631:LEU:CD1    | 2.27                     | 1.22              |
| 10:C16:1348:LEU:HD13 | 10:C16:1359:ILE:CD1 | 1.68                     | 1.22              |
| 14:W:711:ARG:HD2     | 10:C8:1609:ASP:OD2  | 1.29                     | 1.22              |
| 11:A16:35:ARG:NH2    | 22:I:282:GLU:OE1    | 1.70                     | 1.22              |
| 19:4:365:GLU:OE2     | 19:4:442:ARG:NH2    | 1.67                     | 1.22              |
| 21:H24:312:GLN:CG    | 21:H24:316:ILE:HD11 | 1.67                     | 1.22              |
| 7:Q8:343:PRO:O       | 7:Q8:360:ARG:NH2    | 1.72                     | 1.22              |
| 10:C16:65:PRO:HG2    | 10:C16:96:ARG:NH2   | 1.55                     | 1.22              |
| 10:C16:1074:LEU:CD1  | 10:C16:1075:ASP:HA  | 1.68                     | 1.22              |
| 11:A24:388:VAL:H     | 11:A24:459:ARG:NH1  | 1.36                     | 1.22              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C24:65:PRO:HG2   | 10:C24:96:ARG:NH2   | 1.54                     | 1.22              |
| 10:C:1272:GLN:OE1   | 10:C:1289:LYS:HD2   | 1.32                     | 1.22              |
| 11:A32:35:ARG:NH2   | 22:I24:282:GLU:OE1  | 1.70                     | 1.22              |
| 18:B:1156:GLN:HA    | 18:B:1382:LYS:NZ    | 1.55                     | 1.22              |
| 2:M:628:LEU:HD13    | 3:N:223:GLY:O       | 1.35                     | 1.21              |
| 2:M16:844:VAL:HG22  | 4:T16:660:LEU:CD2   | 1.70                     | 1.21              |
| 7:Q16:343:PRO:O     | 7:Q16:360:ARG:NH2   | 1.72                     | 1.21              |
| 10:C24:1166:SER:O   | 10:C24:1168:PRO:HD3 | 1.04                     | 1.21              |
| 11:A40:806:GLN:CD   | 11:A40:847:ARG:HH22 | 1.45                     | 1.21              |
| 10:C:565:ARG:CD     | 10:C:568:TRP:CE3    | 2.22                     | 1.21              |
| 2:M:202:LYS:HE2     | 2:M:206:SER:OG      | 1.41                     | 1.21              |
| 2:M8:399:THR:CB     | 2:M8:480:ARG:HH21   | 1.52                     | 1.21              |
| 2:M16:399:THR:CB    | 2:M16:480:ARG:HH21  | 1.52                     | 1.21              |
| 2:M16:544:LEU:CG    | 2:M16:586:ALA:HB1   | 1.69                     | 1.21              |
| 8:L16:1071:LEU:CD1  | 9:K16:1284:MET:SD   | 2.27                     | 1.21              |
| 10:C16:1272:GLN:OE1 | 10:C16:1289:LYS:HD2 | 1.32                     | 1.21              |
| 13:V:902:MET:CE     | 14:W:777:LEU:CD2    | 2.11                     | 1.21              |
| 10:C8:1010:ALA:N    | 10:C8:1192:ARG:HH22 | 1.37                     | 1.21              |
| 22:I8:131:ARG:HG3   | 23:J8:557:ARG:CZ    | 1.69                     | 1.21              |
| 21:H16:322:LEU:HB3  | 22:I16:300:LEU:CD1  | 1.69                     | 1.21              |
| 14:W:649:LEU:CD2    | 15:J:575:ILE:CD1    | 2.19                     | 1.21              |
| 10:C:65:PRO:HG2     | 10:C:96:ARG:NH2     | 1.54                     | 1.21              |
| 11:A16:388:VAL:H    | 11:A16:459:ARG:NH1  | 1.36                     | 1.21              |
| 11:A32:90:PHE:CE2   | 18:B8:1788:ILE:HG23 | 1.74                     | 1.21              |
| 18:B8:779:LYS:CE    | 18:B8:847:GLN:NE2   | 2.04                     | 1.21              |
| 22:I:131:ARG:HG3    | 23:J32:557:ARG:CZ   | 1.68                     | 1.21              |
| 2:M16:627:TYR:CZ    | 3:N16:166:ALA:O     | 1.94                     | 1.21              |
| 9:K:1248:LEU:HD11   | 9:K:1265:ILE:CD1    | 1.70                     | 1.21              |
| 9:K8:1085:TYR:CZ    | 9:K8:1093:SER:HA    | 1.75                     | 1.21              |
| 10:C16:390:HIS:CE1  | 10:C16:449:GLU:HB3  | 1.76                     | 1.21              |
| 10:C16:1166:SER:O   | 10:C16:1168:PRO:HD3 | 1.04                     | 1.21              |
| 10:C:153:ALA:CB     | 24:D:1403:LEU:CG    | 2.16                     | 1.21              |
| 11:A16:445:ASN:CG   | 17:F8:65:ARG:HH12   | 1.47                     | 1.21              |
| 21:H24:267:LYS:NZ   | 23:J24:631:GLU:OE2  | 1.70                     | 1.21              |
| 10:C32:65:PRO:HG2   | 10:C32:96:ARG:NH2   | 1.54                     | 1.21              |
| 1:R:1326:GLY:HA3    | 10:C:1154:TRP:NE1   | 1.55                     | 1.21              |
| 1:R8:1265:PHE:CE2   | 1:R8:1269:LEU:CD1   | 2.23                     | 1.21              |
| 2:M16:231:ARG:CZ    | 2:M16:299:GLY:HA2   | 1.69                     | 1.21              |
| 9:K8:1248:LEU:HD11  | 9:K8:1265:ILE:CD1   | 1.69                     | 1.21              |
| 18:B8:1110:LEU:CD2  | 21:H24:326:GLY:N    | 2.01                     | 1.21              |
| 1:R8:1449:TRP:CZ3   | 2:M8:160:LEU:CD1    | 2.24                     | 1.20              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:202:LYS:HE2     | 2:M8:206:SER:OG      | 1.41                     | 1.20              |
| 2:M16:672:TYR:CB     | 2:M16:680:LYS:CD     | 2.17                     | 1.20              |
| 8:L8:976:LEU:HD23    | 9:K8:1004:ARG:CD     | 1.57                     | 1.20              |
| 10:C16:390:HIS:HD2   | 10:C16:452:LEU:CB    | 1.50                     | 1.20              |
| 10:C16:667:ILE:CD1   | 10:C16:697:HIS:CE1   | 2.23                     | 1.20              |
| 11:A32:445:ASN:CG    | 17:F24:65:ARG:HH12   | 1.46                     | 1.20              |
| 18:B8:1110:LEU:CD2   | 21:H24:326:GLY:CA    | 2.19                     | 1.20              |
| 22:I16:131:ARG:HG3   | 23:J16:557:ARG:CZ    | 1.69                     | 1.20              |
| 10:C32:1272:GLN:OE1  | 10:C32:1289:LYS:NZ   | 1.75                     | 1.20              |
| 1:R16:1449:TRP:CZ3   | 2:M16:160:LEU:CD1    | 2.24                     | 1.20              |
| 9:K8:1153:ALA:O      | 9:K8:1220:ASN:OD1    | 1.60                     | 1.20              |
| 14:W:631:TYR:CE2     | 15:J:554:LEU:HD21    | 1.75                     | 1.20              |
| 14:W:638:VAL:HG11    | 15:J:561:PHE:CZ      | 1.76                     | 1.20              |
| 10:C:667:ILE:CD1     | 10:C:697:HIS:CE1     | 2.23                     | 1.20              |
| 10:C8:65:PRO:HG2     | 10:C8:96:ARG:NH2     | 1.54                     | 1.20              |
| 18:B:786:ASP:OD2     | 24:D16:1066:VAL:HA   | 1.42                     | 1.20              |
| 21:H:267:LYS:NZ      | 23:J32:631:GLU:OE2   | 1.70                     | 1.20              |
| 1:R:1449:TRP:CZ3     | 2:M:160:LEU:CD1      | 2.24                     | 1.20              |
| 11:A16:676:TYR:CZ    | 24:D16:1395:SER:CA   | 2.20                     | 1.20              |
| 21:H24:160:ARG:NH2   | 21:H24:187:GLU:O     | 1.75                     | 1.20              |
| 1:R8:1124:TRP:CZ2    | 4:T8:669:PRO:HG3     | 1.77                     | 1.20              |
| 2:M16:428:SER:HB2    | 8:L16:355:SER:OG     | 1.11                     | 1.20              |
| 7:Q:343:PRO:O        | 7:Q:360:ARG:NH2      | 1.72                     | 1.20              |
| 10:C24:1547:LYS:HZ3  | 24:D24:1405:GLY:N    | 1.36                     | 1.20              |
| 11:A40:445:ASN:CG    | 17:F16:65:ARG:HH12   | 1.46                     | 1.20              |
| 18:B:1110:LEU:CD2    | 21:H:326:GLY:CA      | 2.19                     | 1.20              |
| 21:H16:139:ASP:OD1   | 21:H16:140:PRO:HD2   | 1.42                     | 1.20              |
| 24:D40:1109:LEU:HD13 | 24:D40:1127:ARG:CG   | 1.72                     | 1.20              |
| 2:M8:428:SER:CB      | 8:L8:355:SER:OG      | 1.89                     | 1.20              |
| 2:M16:351:ALA:HB1    | 8:L16:219:ILE:CG2    | 1.69                     | 1.20              |
| 12:A:153:ARG:HG2     | 10:C8:74:ASP:OD1     | 1.38                     | 1.20              |
| 10:C32:1166:SER:O    | 10:C32:1168:PRO:HD3  | 1.04                     | 1.20              |
| 2:M8:816:ARG:NH1     | 2:M8:849:LEU:HB3     | 1.56                     | 1.19              |
| 2:M16:340:GLU:OE1    | 4:T8:635:ALA:HB1     | 1.40                     | 1.19              |
| 2:M16:833:GLU:OE1    | 4:T16:667:ILE:HA     | 1.37                     | 1.19              |
| 6:O8:119:ARG:NH2     | 6:O8:182:GLU:HG2     | 1.56                     | 1.19              |
| 10:C16:1010:ALA:N    | 10:C16:1192:ARG:HH22 | 1.37                     | 1.19              |
| 10:C24:667:ILE:CD1   | 10:C24:697:HIS:CE1   | 2.23                     | 1.19              |
| 10:C8:1348:LEU:HD13  | 10:C8:1359:ILE:CD1   | 1.68                     | 1.19              |
| 24:D8:857:THR:CG2    | 24:D8:885:TYR:OH     | 1.89                     | 1.19              |
| 2:M8:844:VAL:HG22    | 4:T8:660:LEU:CD2     | 1.70                     | 1.19              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:816:ARG:NH1   | 2:M16:849:LEU:HB3    | 1.56                     | 1.19              |
| 10:C24:407:LYS:CE   | 10:C24:465:PHE:HZ    | 1.48                     | 1.19              |
| 14:W:517:GLU:N      | 14:W:605:ASN:HA      | 0.94                     | 1.19              |
| 10:C:35:ASN:OD1     | 24:D:1148:LEU:CD1    | 1.90                     | 1.19              |
| 11:A16:137:GLU:CG   | 18:B:1901:GLN:HE22   | 1.54                     | 1.19              |
| 18:B:779:LYS:CE     | 18:B:847:GLN:NE2     | 2.04                     | 1.19              |
| 21:H:160:ARG:NH2    | 21:H:187:GLU:O       | 1.75                     | 1.19              |
| 1:R:1428:VAL:CG2    | 6:O:165:LYS:HE3      | 1.69                     | 1.19              |
| 2:M:377:ARG:NH1     | 2:M:477:ASP:HB3      | 1.57                     | 1.19              |
| 6:O16:119:ARG:NH2   | 6:O16:182:GLU:HG2    | 1.56                     | 1.19              |
| 9:K:1085:TYR:CZ     | 9:K:1093:SER:HA      | 1.75                     | 1.19              |
| 9:K:1153:ALA:O      | 9:K:1220:ASN:OD1     | 1.60                     | 1.19              |
| 10:C16:1688:ARG:HG3 | 23:J32:735:LYS:CE    | 1.71                     | 1.19              |
| 10:C16:1699:LYS:NZ  | 23:J32:722:LEU:CD2   | 2.03                     | 1.19              |
| 10:C8:1272:GLN:OE1  | 10:C8:1289:LYS:NZ    | 1.75                     | 1.19              |
| 11:A32:90:PHE:CD2   | 18:B8:1788:ILE:HG23  | 1.78                     | 1.19              |
| 18:B:349:PHE:CE1    | 18:B:353:ILE:HD11    | 1.76                     | 1.19              |
| 18:B8:349:PHE:CE1   | 18:B8:353:ILE:HD11   | 1.76                     | 1.19              |
| 18:B8:1419:LYS:HG3  | 18:B8:1468:PHE:CE1   | 1.77                     | 1.19              |
| 2:M8:833:GLU:OE1    | 4:T8:667:ILE:HA      | 1.37                     | 1.19              |
| 9:K:1085:TYR:OH     | 9:K:1093:SER:HA      | 1.05                     | 1.19              |
| 10:C8:578:LEU:O     | 10:C8:584:ILE:HD12   | 1.43                     | 1.19              |
| 18:B8:1156:GLN:HA   | 18:B8:1382:LYS:NZ    | 1.55                     | 1.19              |
| 21:H16:160:ARG:NH2  | 21:H16:187:GLU:O     | 1.75                     | 1.19              |
| 1:R:1324:ASP:OD1    | 10:C:1180:ILE:HD12   | 1.33                     | 1.19              |
| 1:R16:1124:TRP:CZ2  | 4:T16:669:PRO:HG3    | 1.77                     | 1.19              |
| 10:C24:578:LEU:O    | 10:C24:584:ILE:HD12  | 1.42                     | 1.19              |
| 10:C24:1271:PHE:CE2 | 10:C24:1284:ASP:HB3  | 1.78                     | 1.19              |
| 11:A16:91:GLU:HB3   | 18:B:1112:LYS:HE2    | 1.24                     | 1.19              |
| 18:B:1419:LYS:HG3   | 18:B:1468:PHE:CE1    | 1.77                     | 1.19              |
| 18:B8:1529:GLU:OE2  | 24:D32:1415:LEU:HD11 | 1.26                     | 1.19              |
| 19:4:189:LEU:HD13   | 19:4:203:LEU:CD2     | 1.71                     | 1.19              |
| 21:H8:160:ARG:NH2   | 21:H8:187:GLU:O      | 1.75                     | 1.19              |
| 1:R:768:LEU:HG      | 24:D:1362:VAL:O      | 1.02                     | 1.18              |
| 2:M8:625:HIS:HA     | 3:N8:165:GLY:HA2     | 1.25                     | 1.18              |
| 2:M16:377:ARG:NH1   | 2:M16:477:ASP:HB3    | 1.57                     | 1.18              |
| 6:O:119:ARG:NH2     | 6:O:182:GLU:HG2      | 1.56                     | 1.18              |
| 9:K:847:LEU:HD21    | 9:K:910:SER:OG       | 1.42                     | 1.18              |
| 11:A40:474:LEU:CD1  | 24:D32:1099:ARG:NH2  | 2.05                     | 1.18              |
| 12:A:560:MET:CE     | 12:A:615:GLN:NE2     | 2.07                     | 1.18              |
| 10:C:1272:GLN:OE1   | 10:C:1289:LYS:NZ     | 1.75                     | 1.18              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A16:90:PHE:CD1   | 18:B:1788:ILE:CG2   | 2.20                     | 1.18              |
| 18:B:86:LYS:CG      | 18:B:123:LEU:HD11   | 1.71                     | 1.18              |
| 18:B8:86:LYS:CG     | 18:B8:123:LEU:HD11  | 1.71                     | 1.18              |
| 10:C16:407:LYS:CE   | 10:C16:465:PHE:HZ   | 1.48                     | 1.18              |
| 10:C16:1271:PHE:CE2 | 10:C16:1284:ASP:HB3 | 1.78                     | 1.18              |
| 11:A24:645:GLU:HG2  | 24:D16:867:ASP:CG   | 1.69                     | 1.18              |
| 11:A40:440:LEU:CB   | 11:A40:443:LEU:HD12 | 1.73                     | 1.18              |
| 10:C:1166:SER:O     | 10:C:1168:PRO:HD3   | 1.04                     | 1.18              |
| 10:C:1271:PHE:CE2   | 10:C:1284:ASP:HB3   | 1.78                     | 1.18              |
| 10:C8:1272:GLN:OE1  | 10:C8:1289:LYS:HD2  | 1.32                     | 1.18              |
| 11:A32:137:GLU:CG   | 18:B8:1901:GLN:HE22 | 1.54                     | 1.18              |
| 18:B:786:ASP:OD2    | 24:D16:1066:VAL:CB  | 1.85                     | 1.18              |
| 20:E8:434:TRP:CE2   | 24:D40:72:GLU:HB3   | 1.79                     | 1.18              |
| 21:H:139:ASP:OD1    | 21:H:140:PRO:HD2    | 1.41                     | 1.18              |
| 10:C32:1272:GLN:OE1 | 10:C32:1289:LYS:HD2 | 1.32                     | 1.18              |
| 1:R:1124:TRP:CZ2    | 4:T:669:PRO:HG3     | 1.77                     | 1.18              |
| 10:C16:643:LEU:HD21 | 10:C16:675:ASP:OD2  | 1.02                     | 1.18              |
| 10:C16:1272:GLN:OE1 | 10:C16:1289:LYS:NZ  | 1.75                     | 1.18              |
| 10:C8:1166:SER:O    | 10:C8:1168:PRO:HD3  | 1.04                     | 1.18              |
| 11:A16:212:LYS:HE3  | 11:A16:585:MET:CE   | 1.63                     | 1.18              |
| 18:B:1436:PRO:HB3   | 24:D16:1259:SER:O   | 1.42                     | 1.18              |
| 19:48:189:LEU:HD13  | 19:48:203:LEU:CD2   | 1.71                     | 1.18              |
| 10:C32:499:LEU:HD23 | 10:C32:505:PHE:HE2  | 1.08                     | 1.18              |
| 10:C24:620:PRO:HB3  | 10:C24:636:VAL:CG1  | 1.74                     | 1.18              |
| 12:A:257:GLN:NE2    | 12:A:263:ASP:OD1    | 1.77                     | 1.18              |
| 10:C32:1271:PHE:CE2 | 10:C32:1284:ASP:HB3 | 1.78                     | 1.18              |
| 2:M:672:TYR:CG      | 2:M:680:LYS:NZ      | 2.11                     | 1.18              |
| 1:R8:982:GLU:OE1    | 24:D40:1436:ARG:CB  | 1.90                     | 1.18              |
| 8:L:1081:MET:SD     | 9:K:1083:ILE:HG22   | 1.83                     | 1.18              |
| 9:K:581:ASP:HB3     | 9:K:625:ARG:NH2     | 1.58                     | 1.18              |
| 10:C16:1548:ILE:CD1 | 24:D8:1407:PHE:CE2  | 2.13                     | 1.18              |
| 10:C24:643:LEU:HD21 | 10:C24:675:ASP:OD2  | 1.02                     | 1.18              |
| 10:C24:1272:GLN:OE1 | 10:C24:1289:LYS:NZ  | 1.75                     | 1.18              |
| 11:A40:257:GLN:NE2  | 11:A40:263:ASP:OD1  | 1.77                     | 1.18              |
| 11:A32:326:TYR:CD1  | 17:F24:77:TYR:CB    | 2.27                     | 1.18              |
| 18:B:786:ASP:OD2    | 24:D16:1066:VAL:CA  | 1.92                     | 1.18              |
| 21:H:269:PHE:CE1    | 22:I:205:ARG:NH1    | 2.12                     | 1.18              |
| 21:H24:139:ASP:OD1  | 21:H24:140:PRO:HD2  | 1.42                     | 1.18              |
| 21:H24:269:PHE:CE1  | 22:I24:205:ARG:NH1  | 2.12                     | 1.18              |
| 10:C32:578:LEU:O    | 10:C32:584:ILE:HD12 | 1.42                     | 1.18              |
| 5:P:303:LYS:HE3     | 14:W:84:PRO:O       | 1.43                     | 1.17              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:L16:1030:LEU:CD2  | 9:K16:1285:GLU:OE1  | 1.90                     | 1.17              |
| 9:K:916:LYS:CG      | 9:K:919:MET:CE      | 2.21                     | 1.17              |
| 11:A24:326:TYR:CD1  | 17:F:77:TYR:CB      | 2.27                     | 1.17              |
| 12:A:440:LEU:CB     | 12:A:443:LEU:HD12   | 1.73                     | 1.17              |
| 13:V:787:ILE:HD12   | 15:J:592:VAL:HG13   | 1.25                     | 1.17              |
| 10:C:578:LEU:O      | 10:C:584:ILE:HD12   | 1.43                     | 1.17              |
| 10:C8:1271:PHE:CE2  | 10:C8:1284:ASP:HB3  | 1.78                     | 1.17              |
| 11:A16:257:GLN:NE2  | 11:A16:263:ASP:OD1  | 1.77                     | 1.17              |
| 18:B8:786:ASP:CG    | 24:D32:1066:VAL:CG2 | 2.09                     | 1.17              |
| 18:B8:1436:PRO:HB3  | 24:D32:1259:SER:O   | 1.44                     | 1.17              |
| 1:R:1424:LYS:HD3    | 6:O:107:SER:OG      | 1.44                     | 1.17              |
| 2:M:816:ARG:NH1     | 2:M:849:LEU:HB3     | 1.57                     | 1.17              |
| 1:R16:1078:SER:CB   | 5:P16:713:LEU:HD21  | 1.73                     | 1.17              |
| 5:P:109:ILE:CG1     | 14:W:18:PRO:HG2     | 1.69                     | 1.17              |
| 5:P:318:THR:HG22    | 13:V:763:LYS:NZ     | 1.57                     | 1.17              |
| 7:Q:341:GLN:CG      | 10:C8:751:ARG:NH1   | 1.97                     | 1.17              |
| 9:K8:1085:TYR:HE1   | 9:K8:1093:SER:CB    | 1.42                     | 1.17              |
| 10:C24:848:CYS:HA   | 10:C24:906:ARG:HH22 | 1.09                     | 1.17              |
| 12:A:153:ARG:CG     | 10:C8:74:ASP:OD1    | 1.92                     | 1.17              |
| 10:C:620:PRO:HB3    | 10:C:636:VAL:CG1    | 1.74                     | 1.17              |
| 10:C8:620:PRO:HB3   | 10:C8:636:VAL:CG1   | 1.74                     | 1.17              |
| 10:C32:643:LEU:HD21 | 10:C32:675:ASP:OD2  | 1.02                     | 1.17              |
| 2:M8:627:TYR:HB3    | 3:N8:167:LEU:HD12   | 1.23                     | 1.17              |
| 2:M16:202:LYS:HE2   | 2:M16:206:SER:OG    | 1.41                     | 1.17              |
| 9:K8:847:LEU:HD21   | 9:K8:910:SER:OG     | 1.42                     | 1.17              |
| 10:C16:586:PRO:HD2  | 10:C16:650:ARG:NH1  | 1.60                     | 1.17              |
| 10:C16:1548:ILE:CG1 | 24:D8:1407:PHE:HE2  | 1.57                     | 1.17              |
| 10:C24:453:LEU:HD23 | 10:C24:459:LEU:HD11 | 1.18                     | 1.17              |
| 10:C24:565:ARG:NH2  | 10:C24:569:PHE:HD2  | 1.41                     | 1.17              |
| 10:C:667:ILE:O      | 10:C:668:ALA:C      | 1.68                     | 1.17              |
| 10:C8:586:PRO:HD2   | 10:C8:650:ARG:NH1   | 1.60                     | 1.17              |
| 11:A32:560:MET:CE   | 11:A32:615:GLN:NE2  | 2.07                     | 1.17              |
| 12:A48:440:LEU:CB   | 12:A48:443:LEU:HD12 | 1.73                     | 1.17              |
| 2:M8:377:ARG:NH1    | 2:M8:477:ASP:HB3    | 1.57                     | 1.17              |
| 5:P8:105:ARG:NH1    | 5:P8:130:VAL:HG13   | 1.58                     | 1.17              |
| 9:K:788:LEU:HD22    | 9:K:856:ILE:HD11    | 1.27                     | 1.17              |
| 11:A24:645:GLU:CD   | 24:D16:867:ASP:OD1  | 1.85                     | 1.17              |
| 10:C24:499:LEU:HD23 | 10:C24:505:PHE:HE2  | 1.08                     | 1.17              |
| 10:C:643:LEU:CD1    | 10:C:679:ARG:NH1    | 2.08                     | 1.17              |
| 10:C:643:LEU:HD21   | 10:C:675:ASP:OD2    | 1.02                     | 1.17              |
| 11:A16:560:MET:CE   | 11:A16:615:GLN:NE2  | 2.07                     | 1.17              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R:1360:GLN:HG2    | 10:C:605:GLU:O       | 1.45                     | 1.17              |
| 7:Q8:124:PHE:CD1    | 7:Q8:125:TYR:CZ      | 2.33                     | 1.17              |
| 9:K:1085:TYR:HE1    | 9:K:1093:SER:CB      | 1.42                     | 1.17              |
| 10:C16:643:LEU:CD2  | 10:C16:675:ASP:OD2   | 1.92                     | 1.17              |
| 10:C24:1814:LYS:HE2 | 23:J24:738:MET:SD    | 1.85                     | 1.17              |
| 11:A40:103:GLU:OE1  | 21:H16:323:TYR:OH    | 1.60                     | 1.17              |
| 11:A40:326:TYR:CD1  | 17:F16:77:TYR:CB     | 2.27                     | 1.17              |
| 12:A:212:LYS:HE3    | 12:A:585:MET:CE      | 1.63                     | 1.17              |
| 14:W:627:PHE:CZ     | 15:J:554:LEU:HD13    | 1.79                     | 1.17              |
| 15:J:677:GLY:O      | 15:J:678:GLY:O       | 1.63                     | 1.17              |
| 10:C8:345:MET:CE    | 10:C8:401:ILE:HD13   | 1.75                     | 1.17              |
| 11:A16:326:TYR:CD1  | 17:F8:77:TYR:CB      | 2.27                     | 1.17              |
| 11:A32:440:LEU:CB   | 11:A32:443:LEU:HD12  | 1.73                     | 1.17              |
| 19:48:183:ARG:NH1   | 19:48:245:GLY:HA3    | 1.60                     | 1.17              |
| 21:H:366:MET:CE     | 22:I:332:MET:HE3     | 1.75                     | 1.17              |
| 21:H16:255:LEU:HD12 | 23:J16:655:GLU:OE2   | 1.42                     | 1.17              |
| 21:H16:269:PHE:CE1  | 22:I16:205:ARG:NH1   | 2.12                     | 1.17              |
| 24:D:307:GLY:O      | 24:D16:753:ARG:NH2   | 1.78                     | 1.17              |
| 10:C32:1010:ALA:N   | 10:C32:1192:ARG:HH22 | 1.37                     | 1.17              |
| 2:M:627:TYR:HB3     | 3:N:167:LEU:HD12     | 1.22                     | 1.16              |
| 10:C16:565:ARG:NH2  | 10:C16:569:PHE:HD2   | 1.41                     | 1.16              |
| 11:A40:212:LYS:HE3  | 11:A40:585:MET:CE    | 1.63                     | 1.16              |
| 11:A32:257:GLN:NE2  | 11:A32:263:ASP:OD1   | 1.77                     | 1.16              |
| 18:B8:786:ASP:OD2   | 24:D32:1066:VAL:HG22 | 1.00                     | 1.16              |
| 19:48:357:LYS:NZ    | 19:48:411:LEU:O      | 1.75                     | 1.16              |
| 10:C32:643:LEU:CD2  | 10:C32:675:ASP:OD2   | 1.93                     | 1.16              |
| 8:L:601:HIS:CE1     | 8:L:631:LEU:CD2      | 2.28                     | 1.16              |
| 10:C16:1547:LYS:HZ3 | 24:D8:1405:GLY:N     | 1.41                     | 1.16              |
| 10:C8:499:LEU:HD23  | 10:C8:505:PHE:HE2    | 1.08                     | 1.16              |
| 11:A16:90:PHE:CD2   | 18:B:1788:ILE:HG23   | 1.80                     | 1.16              |
| 11:A32:104:TYR:OH   | 18:B8:1102:LYS:NZ    | 1.78                     | 1.16              |
| 11:A32:154:ILE:CD1  | 18:B8:1842:VAL:HG13  | 1.75                     | 1.16              |
| 19:4:357:LYS:NZ     | 19:4:411:LEU:O       | 1.75                     | 1.16              |
| 20:E8:353:ILE:HD12  | 20:E8:413:PHE:CD2    | 1.79                     | 1.16              |
| 21:H8:269:PHE:CE1   | 22:I8:205:ARG:NH1    | 2.12                     | 1.16              |
| 21:H8:366:MET:CE    | 22:I8:332:MET:HE3    | 1.75                     | 1.16              |
| 12:A48:257:GLN:NE2  | 12:A48:263:ASP:OD1   | 1.77                     | 1.16              |
| 1:R:1269:LEU:CD1    | 5:P:684:ARG:CD       | 2.24                     | 1.16              |
| 1:R8:1466:LYS:CD    | 6:O8:160:LEU:HD22    | 1.74                     | 1.16              |
| 5:P16:112:LEU:HD22  | 5:P16:122:TYR:CD1    | 1.65                     | 1.16              |
| 5:P16:112:LEU:HD21  | 5:P16:122:TYR:CG     | 1.80                     | 1.16              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K8:847:LEU:CD2     | 9:K8:910:SER:OG      | 1.93                     | 1.16              |
| 10:C16:578:LEU:O     | 10:C16:584:ILE:HD12  | 1.43                     | 1.16              |
| 10:C16:668:ALA:HA    | 10:C16:700:MET:HE1   | 1.21                     | 1.16              |
| 11:A24:440:LEU:CB    | 11:A24:443:LEU:HD12  | 1.73                     | 1.16              |
| 11:A40:748:GLU:CB    | 24:D24:1398:ARG:HH12 | 1.58                     | 1.16              |
| 14:W:586:ILE:CD1     | 15:J:572:ASP:HB2     | 1.74                     | 1.16              |
| 11:A16:440:LEU:CB    | 11:A16:443:LEU:HD12  | 1.73                     | 1.16              |
| 18:B:609:TYR:CD2     | 18:B:610:VAL:HG22    | 1.79                     | 1.16              |
| 21:H8:255:LEU:HD12   | 23:J8:655:GLU:OE2    | 1.42                     | 1.16              |
| 21:H16:366:MET:CE    | 22:I16:332:MET:HE3   | 1.75                     | 1.16              |
| 5:P8:55:ARG:NH1      | 5:P8:64:ASP:HB2      | 1.59                     | 1.16              |
| 7:Q16:124:PHE:CD1    | 7:Q16:125:TYR:CZ     | 2.33                     | 1.16              |
| 9:K8:581:ASP:HB3     | 9:K8:625:ARG:NH2     | 1.58                     | 1.16              |
| 10:C16:453:LEU:HD23  | 10:C16:459:LEU:HD11  | 1.17                     | 1.16              |
| 10:C24:643:LEU:CD2   | 10:C24:675:ASP:OD2   | 1.93                     | 1.16              |
| 11:A40:474:LEU:HD13  | 24:D32:1099:ARG:NH1  | 1.60                     | 1.16              |
| 18:B8:609:TYR:CD2    | 18:B8:610:VAL:HG22   | 1.80                     | 1.16              |
| 10:C32:407:LYS:CE    | 10:C32:465:PHE:HZ    | 1.48                     | 1.16              |
| 10:C32:620:PRO:HB3   | 10:C32:636:VAL:CG1   | 1.74                     | 1.16              |
| 10:C32:1348:LEU:HD13 | 10:C32:1359:ILE:CD1  | 1.68                     | 1.16              |
| 4:T16:386:HIS:CD2    | 4:T16:386:HIS:NE2    | 2.13                     | 1.16              |
| 4:T16:386:HIS:CE1    | 4:T16:386:HIS:ND1    | 2.14                     | 1.16              |
| 5:P:55:ARG:NH1       | 5:P:64:ASP:HB2       | 1.59                     | 1.16              |
| 8:L8:270:LEU:CD2     | 12:A48:155:SER:CB    | 2.23                     | 1.16              |
| 9:K:847:LEU:CD2      | 9:K:910:SER:OG       | 1.93                     | 1.16              |
| 10:C16:620:PRO:HB3   | 10:C16:636:VAL:CG1   | 1.74                     | 1.16              |
| 11:A24:465:SER:HB3   | 24:D16:1100:GLN:HE22 | 1.03                     | 1.16              |
| 10:C24:407:LYS:CE    | 10:C24:465:PHE:CE2   | 2.26                     | 1.16              |
| 10:C24:668:ALA:HA    | 10:C24:700:MET:HE1   | 1.21                     | 1.16              |
| 10:C24:1708:ARG:NH1  | 21:H24:279:GLU:CD    | 2.01                     | 1.16              |
| 14:W:715:ASP:OD1     | 10:C8:1568:ARG:CD    | 1.93                     | 1.16              |
| 10:C:586:PRO:HD2     | 10:C:650:ARG:NH1     | 1.60                     | 1.16              |
| 20:E:353:ILE:HD12    | 20:E:413:PHE:CD2     | 1.79                     | 1.16              |
| 21:H:255:LEU:HD12    | 23:J32:655:GLU:OE2   | 1.42                     | 1.16              |
| 21:H8:139:ASP:OD1    | 21:H8:140:PRO:HD2    | 1.42                     | 1.16              |
| 21:H24:255:LEU:HD12  | 23:J24:655:GLU:OE2   | 1.42                     | 1.16              |
| 4:T8:386:HIS:ND1     | 4:T8:386:HIS:CE1     | 2.14                     | 1.15              |
| 5:P:398:LYS:HB2      | 5:P:426:MET:CE       | 1.76                     | 1.15              |
| 5:P16:57:PRO:HB2     | 6:O16:29:LEU:HD11    | 1.20                     | 1.15              |
| 12:A:642:GLY:CA      | 12:A:685:ARG:NH2     | 2.08                     | 1.15              |
| 10:C:1348:LEU:HD13   | 10:C:1359:ILE:CD1    | 1.68                     | 1.15              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 11:A16:104:TYR:OH  | 18:B:1102:LYS:NZ     | 1.78                     | 1.15              |
| 18:B:1768:ILE:HG22 | 18:B:1770:THR:HG22   | 1.21                     | 1.15              |
| 2:M:202:LYS:CE     | 2:M:206:SER:OG       | 1.95                     | 1.15              |
| 3:N16:4:GLN:HE22   | 3:N16:44:GLY:HA2     | 1.11                     | 1.15              |
| 5:P:109:ILE:CD1    | 14:W:18:PRO:CG       | 2.25                     | 1.15              |
| 12:A:440:LEU:HB2   | 12:A:443:LEU:HD12    | 1.24                     | 1.15              |
| 14:W:586:ILE:HD11  | 15:J:572:ASP:HB2     | 1.24                     | 1.15              |
| 10:C:565:ARG:NH2   | 10:C:569:PHE:HD2     | 1.40                     | 1.15              |
| 10:C8:572:ILE:CD1  | 10:C8:606:MET:CE     | 2.24                     | 1.15              |
| 24:D:400:VAL:HB    | 24:D16:751:MET:CE    | 1.76                     | 1.15              |
| 24:D:403:ARG:HB3   | 24:D16:748:GLU:OE1   | 1.44                     | 1.15              |
| 10:C32:228:ARG:NH2 | 10:C32:277:SER:OG    | 1.80                     | 1.15              |
| 10:C32:586:PRO:HD2 | 10:C32:650:ARG:NH1   | 1.60                     | 1.15              |
| 3:N8:162:THR:HG23  | 3:N8:168:VAL:HG22    | 1.29                     | 1.15              |
| 3:N16:208:LYS:NZ   | 3:N16:252:GLY:O      | 1.80                     | 1.15              |
| 5:P:322:CYS:O      | 13:V:767:GLU:OE2     | 1.62                     | 1.15              |
| 8:L16:1026:ARG:HD2 | 9:K16:1284:MET:HG2   | 1.22                     | 1.15              |
| 9:K8:788:LEU:HD22  | 9:K8:856:ILE:HD11    | 1.27                     | 1.15              |
| 10:C16:848:CYS:HA  | 10:C16:906:ARG:HH22  | 1.09                     | 1.15              |
| 11:A24:257:GLN:NE2 | 11:A24:263:ASP:OD1   | 1.77                     | 1.15              |
| 11:A24:560:MET:CE  | 11:A24:615:GLN:NE2   | 2.07                     | 1.15              |
| 11:A40:560:MET:CE  | 11:A40:615:GLN:NE2   | 2.07                     | 1.15              |
| 10:C:668:ALA:HA    | 10:C:700:MET:CE      | 1.77                     | 1.15              |
| 11:A16:154:ILE:CD1 | 18:B:1842:VAL:HG13   | 1.75                     | 1.15              |
| 20:E:355:PRO:HA    | 20:E:454:MET:HE1     | 1.15                     | 1.15              |
| 21:H8:231:HIS:CD2  | 23:J8:596:GLN:HE21   | 1.57                     | 1.15              |
| 12:A48:440:LEU:HB2 | 12:A48:443:LEU:CD1   | 1.77                     | 1.15              |
| 2:M16:544:LEU:HD11 | 2:M16:586:ALA:O      | 1.47                     | 1.15              |
| 4:T8:386:HIS:NE2   | 4:T8:386:HIS:CD2     | 2.13                     | 1.15              |
| 9:K:916:LYS:O      | 9:K:919:MET:HG2      | 1.47                     | 1.15              |
| 9:K8:1085:TYR:CE1  | 9:K8:1093:SER:CA     | 2.29                     | 1.15              |
| 10:C16:668:ALA:HA  | 10:C16:700:MET:CE    | 1.77                     | 1.15              |
| 10:C16:1664:SER:N  | 10:C24:1568:ARG:HH21 | 1.43                     | 1.15              |
| 10:C24:586:PRO:HD2 | 10:C24:650:ARG:NH1   | 1.60                     | 1.15              |
| 14:W:513:SER:O     | 14:W:607:ARG:NH1     | 1.77                     | 1.15              |
| 14:W:711:ARG:HH11  | 10:C8:1609:ASP:CB    | 1.58                     | 1.15              |
| 10:C:345:MET:CE    | 10:C:401:ILE:HD13    | 1.75                     | 1.15              |
| 18:B:583:ARG:NH1   | 18:B:711:CYS:HB2     | 1.61                     | 1.15              |
| 1:R8:1188:TYR:CZ   | 24:D40:1459:LEU:HB3  | 1.81                     | 1.15              |
| 1:R8:1466:LYS:CB   | 6:O8:160:LEU:HD13    | 1.76                     | 1.15              |
| 4:T:386:HIS:NE2    | 4:T:386:HIS:CD2      | 2.13                     | 1.15              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 5:P:398:LYS:CB      | 5:P:426:MET:HE2      | 1.76                     | 1.15              |
| 9:K:1085:TYR:CE1    | 9:K:1093:SER:CA      | 2.29                     | 1.15              |
| 9:K8:788:LEU:CD2    | 9:K8:856:ILE:HD11    | 1.77                     | 1.15              |
| 10:C16:228:ARG:NH2  | 10:C16:277:SER:OG    | 1.80                     | 1.15              |
| 10:C16:1664:SER:N   | 10:C24:1568:ARG:NH2  | 1.93                     | 1.15              |
| 10:C24:228:ARG:NH2  | 10:C24:277:SER:OG    | 1.80                     | 1.15              |
| 10:C:643:LEU:CD2    | 10:C:675:ASP:OD2     | 1.92                     | 1.15              |
| 10:C8:228:ARG:NH2   | 10:C8:277:SER:OG     | 1.80                     | 1.15              |
| 18:B8:786:ASP:CG    | 24:D32:1066:VAL:HG13 | 1.72                     | 1.15              |
| 19:48:189:LEU:HD13  | 19:48:203:LEU:HD23   | 1.28                     | 1.15              |
| 10:C32:643:LEU:CD1  | 10:C32:679:ARG:NH1   | 2.08                     | 1.15              |
| 5:P16:101:LEU:HD23  | 5:P16:133:TYR:OH     | 1.45                     | 1.14              |
| 10:C24:572:ILE:CD1  | 10:C24:606:MET:CE    | 2.24                     | 1.14              |
| 12:A:440:LEU:HB2    | 12:A:443:LEU:CD1     | 1.77                     | 1.14              |
| 10:C:1265:ARG:O     | 10:C:1268:ARG:HG2    | 1.35                     | 1.14              |
| 10:C:1703:ILE:HD12  | 10:C:1741:MET:HE1    | 1.29                     | 1.14              |
| 20:E8:434:TRP:CD1   | 24:D40:72:GLU:HB3    | 1.82                     | 1.14              |
| 21:H24:366:MET:CE   | 22:I24:332:MET:HE3   | 1.75                     | 1.14              |
| 10:C32:407:LYS:CE   | 10:C32:465:PHE:CE2   | 2.26                     | 1.14              |
| 10:C32:668:ALA:HA   | 10:C32:700:MET:CE    | 1.77                     | 1.14              |
| 12:A48:560:MET:CE   | 12:A48:615:GLN:NE2   | 2.07                     | 1.14              |
| 1:R:1324:ASP:OD2    | 10:C:1180:ILE:CG2    | 1.96                     | 1.14              |
| 1:R:1330:ALA:HB3    | 10:C:1173:LEU:CD1    | 1.77                     | 1.14              |
| 4:T:386:HIS:ND1     | 4:T:386:HIS:CE1      | 2.14                     | 1.14              |
| 5:P:109:ILE:CG2     | 14:W:18:PRO:HG2      | 1.76                     | 1.14              |
| 5:P:600:PHE:CD2     | 5:P:638:SER:OG       | 1.83                     | 1.14              |
| 5:P8:614:VAL:H      | 5:P8:629:ARG:NH2     | 1.44                     | 1.14              |
| 5:P16:55:ARG:NH1    | 5:P16:64:ASP:HB2     | 1.59                     | 1.14              |
| 8:L16:1034:VAL:HG21 | 8:L16:1068:PHE:CE2   | 1.82                     | 1.14              |
| 9:K:788:LEU:CD2     | 9:K:856:ILE:HD11     | 1.77                     | 1.14              |
| 9:K8:1248:LEU:HD11  | 9:K8:1265:ILE:HD11   | 1.15                     | 1.14              |
| 10:C24:1010:ALA:N   | 10:C24:1192:ARG:HH22 | 1.37                     | 1.14              |
| 11:A40:440:LEU:HB2  | 11:A40:443:LEU:CD1   | 1.77                     | 1.14              |
| 14:W:638:VAL:HG11   | 15:J:561:PHE:CE2     | 1.82                     | 1.14              |
| 14:W:649:LEU:HD23   | 15:J:575:ILE:HD13    | 1.27                     | 1.14              |
| 11:A32:122:LYS:HE3  | 18:B8:1757:GLU:CD    | 1.71                     | 1.14              |
| 18:B:457:SER:HA     | 18:B:548:ARG:NH1     | 1.62                     | 1.14              |
| 18:B8:583:ARG:NH1   | 18:B8:711:CYS:HB2    | 1.61                     | 1.14              |
| 19:4:183:ARG:HH12   | 19:4:245:GLY:HA3     | 0.98                     | 1.14              |
| 1:R:1269:LEU:HD13   | 5:P:684:ARG:CD       | 1.78                     | 1.14              |
| 2:M:625:HIS:HA      | 3:N:165:GLY:HA2      | 1.26                     | 1.14              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M:672:TYR:HB3      | 2:M:680:LYS:CD      | 1.77                     | 1.14              |
| 2:M:844:VAL:HG22     | 4:T:660:LEU:CD2     | 1.75                     | 1.14              |
| 1:R8:1185:THR:HG21   | 24:D40:1462:PHE:HZ  | 0.97                     | 1.14              |
| 1:R8:1434:VAL:HG13   | 2:M8:176:VAL:HG22   | 1.24                     | 1.14              |
| 5:P:595:SER:C        | 5:P:597:GLY:H       | 1.55                     | 1.14              |
| 7:Q:124:PHE:CD1      | 7:Q:125:TYR:CZ      | 2.33                     | 1.14              |
| 5:P8:101:LEU:HD23    | 5:P8:133:TYR:CZ     | 1.83                     | 1.14              |
| 5:P8:611:LEU:HA      | 5:P8:629:ARG:CZ     | 1.75                     | 1.14              |
| 5:P16:595:SER:C      | 5:P16:597:GLY:H     | 1.55                     | 1.14              |
| 9:K:635:ALA:CB       | 9:K:655:GLN:NE2     | 2.10                     | 1.14              |
| 10:C24:1547:LYS:HD3  | 24:D24:1406:SER:H   | 1.06                     | 1.14              |
| 14:W:513:SER:C       | 14:W:607:ARG:NH1    | 2.02                     | 1.14              |
| 11:A32:104:TYR:OH    | 18:B8:1354:ASP:OD2  | 1.66                     | 1.14              |
| 10:C32:848:CYS:HA    | 10:C32:906:ARG:HH22 | 1.09                     | 1.14              |
| 2:M:377:ARG:NH1      | 2:M:477:ASP:CB      | 2.11                     | 1.14              |
| 3:N:208:LYS:NZ       | 3:N:252:GLY:O       | 1.80                     | 1.14              |
| 2:M16:202:LYS:CE     | 2:M16:206:SER:OG    | 1.95                     | 1.14              |
| 10:C16:572:ILE:CD1   | 10:C16:606:MET:CE   | 2.24                     | 1.14              |
| 10:C24:345:MET:CE    | 10:C24:401:ILE:HD13 | 1.75                     | 1.14              |
| 10:C24:1688:ARG:HG3  | 23:J24:735:LYS:CE   | 1.77                     | 1.14              |
| 11:A40:468:VAL:HG21  | 24:D32:1100:GLN:CD  | 1.73                     | 1.14              |
| 12:A:707:LEU:HG      | 12:A:767:ARG:HH22   | 1.12                     | 1.14              |
| 10:C:667:ILE:HD13    | 10:C:697:HIS:HE1    | 1.08                     | 1.14              |
| 11:A32:519:MET:CE    | 11:A32:569:MET:HE1  | 1.78                     | 1.14              |
| 19:4:183:ARG:NH1     | 19:4:245:GLY:HA3    | 1.60                     | 1.14              |
| 24:D40:1109:LEU:CD1  | 24:D40:1127:ARG:HG3 | 1.78                     | 1.14              |
| 10:C32:1703:ILE:HD12 | 10:C32:1741:MET:HE1 | 1.29                     | 1.14              |
| 1:R8:983:ARG:O       | 24:D40:1360:ALA:HB1 | 1.34                     | 1.14              |
| 1:R8:1059:ILE:HG21   | 24:D40:1435:ARG:NH2 | 0.81                     | 1.14              |
| 2:M8:202:LYS:CE      | 2:M8:206:SER:OG     | 1.95                     | 1.14              |
| 2:M16:377:ARG:NH1    | 2:M16:477:ASP:CB    | 2.11                     | 1.14              |
| 9:K8:635:ALA:CB      | 9:K8:655:GLN:NE2    | 2.10                     | 1.14              |
| 10:C16:1265:ARG:O    | 10:C16:1268:ARG:HG2 | 1.35                     | 1.14              |
| 10:C16:1664:SER:HA   | 10:C24:1568:ARG:NH2 | 1.62                     | 1.14              |
| 11:A24:519:MET:HE1   | 11:A24:569:MET:HE3  | 1.15                     | 1.14              |
| 10:C24:1272:GLN:OE1  | 10:C24:1289:LYS:CE  | 1.95                     | 1.14              |
| 10:C8:848:CYS:HA     | 10:C8:906:ARG:HH22  | 1.09                     | 1.14              |
| 11:A16:440:LEU:HB2   | 11:A16:443:LEU:CD1  | 1.77                     | 1.14              |
| 24:D40:839:GLU:CB    | 24:D40:971:HIS:CE1  | 2.30                     | 1.14              |
| 3:N8:208:LYS:NZ      | 3:N8:252:GLY:O      | 1.80                     | 1.13              |
| 2:M16:627:TYR:HB3    | 3:N16:167:LEU:HD12  | 1.21                     | 1.13              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:667:ILE:HD13  | 10:C16:697:HIS:HE1  | 1.09                     | 1.13              |
| 11:A40:519:MET:HE1   | 11:A40:569:MET:HE3  | 1.15                     | 1.13              |
| 12:A:560:MET:HE1     | 12:A:615:GLN:HE22   | 1.05                     | 1.13              |
| 10:C:228:ARG:NH2     | 10:C:277:SER:OG     | 1.80                     | 1.13              |
| 10:C:627:VAL:HG12    | 10:C:628:GLY:H      | 1.11                     | 1.13              |
| 11:A16:440:LEU:HB2   | 11:A16:443:LEU:HD12 | 1.24                     | 1.13              |
| 11:A32:707:LEU:HB2   | 24:D32:1398:ARG:NH2 | 1.62                     | 1.13              |
| 2:M16:762:LEU:CB     | 2:M16:813:ASN:ND2   | 2.10                     | 1.13              |
| 6:O:82:LEU:HD23      | 6:O:103:MET:CE      | 1.78                     | 1.13              |
| 9:K:1019:ARG:NE      | 9:K:1059:ARG:HD3    | 1.63                     | 1.13              |
| 10:C16:1163:LEU:HD23 | 10:C16:1166:SER:OG  | 1.48                     | 1.13              |
| 10:C16:1272:GLN:OE1  | 10:C16:1289:LYS:CE  | 1.96                     | 1.13              |
| 11:A24:390:ALA:CB    | 24:D16:1099:ARG:HB2 | 1.77                     | 1.13              |
| 11:A24:440:LEU:HB2   | 11:A24:443:LEU:CD1  | 1.77                     | 1.13              |
| 10:C24:557:VAL:CG2   | 10:C24:565:ARG:HH21 | 1.61                     | 1.13              |
| 10:C24:668:ALA:HA    | 10:C24:700:MET:CE   | 1.77                     | 1.13              |
| 10:C24:1163:LEU:HD23 | 10:C24:1166:SER:OG  | 1.48                     | 1.13              |
| 11:A40:440:LEU:HB2   | 11:A40:443:LEU:HD12 | 1.24                     | 1.13              |
| 11:A40:519:MET:CE    | 11:A40:569:MET:HE1  | 1.78                     | 1.13              |
| 10:C:668:ALA:HA      | 10:C:700:MET:HE1    | 1.21                     | 1.13              |
| 11:A16:90:PHE:CZ     | 18:B:1788:ILE:HG23  | 1.83                     | 1.13              |
| 11:A16:104:TYR:OH    | 18:B:1354:ASP:OD2   | 1.66                     | 1.13              |
| 11:A32:121:GLN:HE22  | 18:B8:1559:ALA:CB   | 1.60                     | 1.13              |
| 11:A32:440:LEU:HB2   | 11:A32:443:LEU:CD1  | 1.77                     | 1.13              |
| 20:E8:432:ILE:HD12   | 24:D40:72:GLU:HG3   | 1.22                     | 1.13              |
| 21:H16:231:HIS:CD2   | 23:J16:596:GLN:HE21 | 1.57                     | 1.13              |
| 24:D:405:GLN:CG      | 24:D16:10:ARG:HH11  | 1.50                     | 1.13              |
| 10:C32:1265:ARG:O    | 10:C32:1268:ARG:HG2 | 1.35                     | 1.13              |
| 12:A48:560:MET:HE1   | 12:A48:615:GLN:HE22 | 1.05                     | 1.13              |
| 2:M:762:LEU:CB       | 2:M:813:ASN:ND2     | 2.10                     | 1.13              |
| 3:N16:162:THR:HG21   | 3:N16:168:VAL:HG23  | 1.14                     | 1.13              |
| 6:O8:82:LEU:HD23     | 6:O8:103:MET:CE     | 1.78                     | 1.13              |
| 8:L16:856:LEU:HD23   | 9:K16:1281:SER:OG   | 1.49                     | 1.13              |
| 9:K8:958:MET:CE      | 9:K8:974:LEU:HD22   | 1.78                     | 1.13              |
| 10:C16:1699:LYS:HZ1  | 23:J32:722:LEU:CD2  | 1.60                     | 1.13              |
| 10:C24:390:HIS:HB3   | 10:C24:452:LEU:CD2  | 1.76                     | 1.13              |
| 10:C8:668:ALA:HA     | 10:C8:700:MET:CE    | 1.77                     | 1.13              |
| 11:A16:122:LYS:HE3   | 18:B:1757:GLU:CD    | 1.70                     | 1.13              |
| 18:B:782:THR:O       | 24:D16:1066:VAL:CG2 | 1.96                     | 1.13              |
| 19:48:183:ARG:HH12   | 19:48:245:GLY:HA3   | 0.98                     | 1.13              |
| 20:E8:353:ILE:HG21   | 20:E8:413:PHE:CE2   | 1.84                     | 1.13              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C32:407:LYS:CG   | 10:C32:465:PHE:HZ   | 1.62                     | 1.13              |
| 2:M16:540:TYR:CD1   | 2:M16:555:LEU:HD22  | 1.60                     | 1.13              |
| 2:M16:672:TYR:CE1   | 2:M16:680:LYS:NZ    | 2.15                     | 1.13              |
| 5:P16:527:LYS:CE    | 6:O16:68:GLU:OE1    | 1.97                     | 1.13              |
| 9:K:1248:LEU:HD11   | 9:K:1265:ILE:HD11   | 1.15                     | 1.13              |
| 9:K8:634:LEU:HD22   | 9:K8:754:ARG:HH12   | 1.12                     | 1.13              |
| 11:A24:519:MET:CE   | 11:A24:569:MET:HE1  | 1.78                     | 1.13              |
| 12:A:519:MET:CE     | 12:A:569:MET:HE1    | 1.78                     | 1.13              |
| 18:B:786:ASP:CG     | 24:D16:1066:VAL:CG2 | 2.10                     | 1.13              |
| 24:D:405:GLN:OE1    | 24:D16:10:ARG:CG    | 1.96                     | 1.13              |
| 2:M8:377:ARG:NH1    | 2:M8:477:ASP:CB     | 2.11                     | 1.12              |
| 2:M8:762:LEU:CB     | 2:M8:813:ASN:ND2    | 2.10                     | 1.12              |
| 5:P8:592:SER:OG     | 5:P8:598:LEU:HD13   | 1.49                     | 1.12              |
| 8:L8:1077:LEU:HD13  | 9:K8:1086:VAL:CG1   | 1.77                     | 1.12              |
| 10:C24:1265:ARG:O   | 10:C24:1268:ARG:HG2 | 1.35                     | 1.13              |
| 10:C24:1453:ARG:NH2 | 24:D24:1150:GLY:CA  | 1.86                     | 1.12              |
| 14:W:517:GLU:H      | 14:W:605:ASN:CA     | 1.44                     | 1.13              |
| 10:C:323:HIS:CE1    | 10:C:327:ILE:HD11   | 1.84                     | 1.12              |
| 10:C:1010:ALA:N     | 10:C:1192:ARG:HH22  | 1.37                     | 1.12              |
| 18:B:191:PHE:CZ     | 18:B:193:LYS:HA     | 1.84                     | 1.13              |
| 18:B:779:LYS:CE     | 18:B:847:GLN:HE21   | 1.62                     | 1.13              |
| 18:B:1112:LYS:CE    | 21:H:327:SER:C      | 2.22                     | 1.13              |
| 10:C16:557:VAL:CG2  | 10:C16:565:ARG:HH21 | 1.61                     | 1.12              |
| 11:A40:560:MET:HE1  | 11:A40:615:GLN:HE22 | 1.05                     | 1.12              |
| 18:B8:191:PHE:CZ    | 18:B8:193:LYS:HA    | 1.84                     | 1.12              |
| 21:H:322:LEU:CB     | 22:I:300:LEU:HD11   | 1.79                     | 1.12              |
| 10:C32:1272:GLN:OE1 | 10:C32:1289:LYS:CE  | 1.95                     | 1.12              |
| 1:R:1187:ARG:HH22   | 1:R:1201:LEU:HD11   | 0.97                     | 1.12              |
| 1:R16:1078:SER:OG   | 5:P16:713:LEU:CD2   | 1.97                     | 1.12              |
| 5:P:251:LYS:HE3     | 14:W:765:LYS:HE2    | 1.25                     | 1.12              |
| 5:P8:527:LYS:CE     | 6:O8:68:GLU:OE1     | 1.97                     | 1.12              |
| 11:A24:440:LEU:HB2  | 11:A24:443:LEU:HD12 | 1.24                     | 1.12              |
| 14:W:649:LEU:HD21   | 15:J:575:ILE:HD12   | 1.30                     | 1.12              |
| 10:C:572:ILE:CD1    | 10:C:606:MET:CE     | 2.24                     | 1.12              |
| 11:A16:121:GLN:HE22 | 18:B:1559:ALA:CB    | 1.60                     | 1.12              |
| 11:A32:676:TYR:CE2  | 24:D32:1396:PRO:HD2 | 1.82                     | 1.12              |
| 18:B:1342:LEU:HD23  | 18:B:1406:ALA:HB1   | 1.32                     | 1.12              |
| 18:B8:779:LYS:CE    | 18:B8:847:GLN:HE21  | 1.61                     | 1.12              |
| 18:B8:1768:ILE:HG22 | 18:B8:1770:THR:HG22 | 1.21                     | 1.12              |
| 24:D40:873:ARG:NH1  | 24:D40:884:ASP:CB   | 2.11                     | 1.12              |
| 12:A48:707:LEU:HG   | 12:A48:767:ARG:HH22 | 1.12                     | 1.12              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:625:HIS:HA    | 3:N16:165:GLY:HA2    | 1.26                     | 1.12              |
| 9:K:958:MET:CE      | 9:K:974:LEU:HD22     | 1.78                     | 1.12              |
| 10:C16:345:MET:HE1  | 10:C16:401:ILE:HD12  | 1.26                     | 1.12              |
| 10:C16:345:MET:CE   | 10:C16:401:ILE:HD13  | 1.75                     | 1.12              |
| 10:C16:407:LYS:CG   | 10:C16:465:PHE:HZ    | 1.62                     | 1.12              |
| 10:C:62:ILE:HD12    | 10:C:72:LEU:HD11     | 1.31                     | 1.12              |
| 10:C:557:VAL:CG2    | 10:C:565:ARG:HH21    | 1.62                     | 1.12              |
| 10:C8:643:LEU:HB3   | 10:C8:679:ARG:HH22   | 1.15                     | 1.12              |
| 21:H:291:VAL:HG12   | 23:J32:657:GLU:HG2   | 1.17                     | 1.12              |
| 21:H:363:MET:SD     | 22:I:332:MET:HE1     | 1.90                     | 1.12              |
| 2:M16:185:ARG:NH1   | 2:M16:213:LEU:CD1    | 2.13                     | 1.12              |
| 5:P:527:LYS:CE      | 6:O:68:GLU:OE1       | 1.97                     | 1.12              |
| 8:L16:1030:LEU:HD22 | 9:K16:1285:GLU:OE1   | 0.96                     | 1.12              |
| 10:C16:565:ARG:HD3  | 10:C16:568:TRP:CE3   | 1.84                     | 1.12              |
| 10:C16:1664:SER:CA  | 10:C24:1568:ARG:NH2  | 2.12                     | 1.12              |
| 10:C24:407:LYS:CG   | 10:C24:465:PHE:HZ    | 1.62                     | 1.12              |
| 10:C24:1708:ARG:NE  | 21:H24:279:GLU:OE1   | 1.74                     | 1.12              |
| 10:C8:1272:GLN:OE1  | 10:C8:1289:LYS:CE    | 1.96                     | 1.12              |
| 20:E8:355:PRO:HA    | 20:E8:454:MET:HE1    | 1.15                     | 1.12              |
| 21:H8:322:LEU:CB    | 22:I8:300:LEU:HD11   | 1.79                     | 1.12              |
| 1:R8:1266:THR:CA    | 5:P8:684:ARG:HH21    | 1.61                     | 1.12              |
| 8:L16:1041:SER:CB   | 8:L16:1054:HIS:CE1   | 2.33                     | 1.12              |
| 10:C16:323:HIS:CE1  | 10:C16:327:ILE:HD11  | 1.85                     | 1.12              |
| 10:C24:62:ILE:HD12  | 10:C24:72:LEU:HD11   | 1.31                     | 1.12              |
| 10:C24:557:VAL:HG22 | 10:C24:565:ARG:NH2   | 1.65                     | 1.12              |
| 10:C:35:ASN:HA      | 24:D:1148:LEU:HD11   | 1.26                     | 1.12              |
| 10:C:153:ALA:HB3    | 24:D:1403:LEU:HG     | 1.17                     | 1.12              |
| 10:C8:323:HIS:CE1   | 10:C8:327:ILE:HD11   | 1.85                     | 1.12              |
| 20:E:429:PRO:HG3    | 24:D:69:VAL:HA       | 1.32                     | 1.12              |
| 20:E8:352:PHE:CE1   | 20:E8:451:ILE:CD1    | 2.33                     | 1.12              |
| 21:H:231:HIS:CD2    | 23:J32:596:GLN:HE21  | 1.57                     | 1.12              |
| 21:H16:322:LEU:CB   | 22:I16:300:LEU:HD11  | 1.79                     | 1.12              |
| 2:M:185:ARG:NH1     | 2:M:213:LEU:CD1      | 2.13                     | 1.11              |
| 2:M:672:TYR:CB      | 2:M:680:LYS:CD       | 2.27                     | 1.11              |
| 2:M8:672:TYR:HB3    | 2:M8:680:LYS:CD      | 1.44                     | 1.11              |
| 5:P16:112:LEU:HD21  | 5:P16:122:TYR:CD1    | 1.70                     | 1.11              |
| 10:C24:627:VAL:HG12 | 10:C24:628:GLY:H     | 1.11                     | 1.11              |
| 18:B:782:THR:O      | 24:D16:1066:VAL:HG21 | 1.47                     | 1.11              |
| 18:B:1205:ILE:HD11  | 18:B:1271:PHE:CD2    | 1.86                     | 1.11              |
| 22:I24:199:PHE:CB   | 23:J24:620:MET:SD    | 2.38                     | 1.11              |
| 12:A48:519:MET:CE   | 12:A48:569:MET:HE1   | 1.78                     | 1.11              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 1:R16:1078:SER:HB2   | 5:P16:713:LEU:HD21  | 1.32                     | 1.11              |
| 2:M16:401:ARG:HH22   | 8:L16:381:GLU:HB3   | 1.00                     | 1.11              |
| 11:A40:440:LEU:CB    | 11:A40:443:LEU:CD1  | 2.29                     | 1.11              |
| 10:C8:668:ALA:HA     | 10:C8:700:MET:HE1   | 1.21                     | 1.11              |
| 11:A16:90:PHE:CE2    | 18:B:1788:ILE:CG2   | 2.33                     | 1.11              |
| 11:A32:90:PHE:CE1    | 18:B8:1788:ILE:CG2  | 2.32                     | 1.11              |
| 11:A32:137:GLU:HG3   | 18:B8:1901:GLN:NE2  | 1.64                     | 1.11              |
| 18:B:1130:LEU:HD23   | 18:B:1132:TRP:NE1   | 1.65                     | 1.11              |
| 19:48:252:ARG:CG     | 19:48:281:TRP:HH2   | 1.63                     | 1.11              |
| 10:C32:323:HIS:CE1   | 10:C32:327:ILE:HD11 | 1.84                     | 1.11              |
| 12:A48:440:LEU:CB    | 12:A48:443:LEU:CD1  | 2.29                     | 1.11              |
| 2:M8:185:ARG:NH1     | 2:M8:213:LEU:CD1    | 2.13                     | 1.11              |
| 5:P:57:PRO:HB2       | 6:O:29:LEU:HD11     | 1.20                     | 1.11              |
| 5:P:592:SER:OG       | 5:P:598:LEU:HD13    | 1.49                     | 1.11              |
| 5:P16:592:SER:OG     | 5:P16:598:LEU:HD13  | 1.49                     | 1.11              |
| 7:Q16:143:ARG:NH2    | 7:Q16:147:GLU:OE2   | 1.84                     | 1.11              |
| 8:L:1041:SER:CB      | 8:L:1054:HIS:CE1    | 2.33                     | 1.11              |
| 11:A24:707:LEU:HG    | 11:A24:767:ARG:NH2  | 1.66                     | 1.11              |
| 12:A:707:LEU:HG      | 12:A:767:ARG:NH2    | 1.66                     | 1.11              |
| 13:V:794:ILE:HD12    | 15:J:599:LEU:HD22   | 1.11                     | 1.11              |
| 14:W:586:ILE:HD11    | 15:J:572:ASP:CB     | 1.79                     | 1.11              |
| 10:C:499:LEU:HD23    | 10:C:505:PHE:CE2    | 1.86                     | 1.11              |
| 10:C:1272:GLN:OE1    | 10:C:1289:LYS:CE    | 1.96                     | 1.11              |
| 11:A16:519:MET:CE    | 11:A16:569:MET:HE1  | 1.78                     | 1.11              |
| 18:B8:457:SER:HA     | 18:B8:548:ARG:NH1   | 1.62                     | 1.11              |
| 22:I:199:PHE:CB      | 23:J32:620:MET:SD   | 2.38                     | 1.11              |
| 21:H24:363:MET:SD    | 22:I24:332:MET:HE1  | 1.90                     | 1.11              |
| 24:D40:839:GLU:HB3   | 24:D40:971:HIS:NE2  | 1.65                     | 1.11              |
| 10:C32:1163:LEU:HD23 | 10:C32:1166:SER:OG  | 1.47                     | 1.11              |
| 1:R:979:GLN:OE1      | 24:D:1438:ALA:N     | 1.84                     | 1.11              |
| 3:N:4:GLN:HE22       | 3:N:44:GLY:HA2      | 1.11                     | 1.11              |
| 2:M16:540:TYR:CD1    | 2:M16:555:LEU:HD21  | 1.85                     | 1.11              |
| 5:P:152:ILE:CG2      | 14:W:762:GLN:NE2    | 2.14                     | 1.11              |
| 5:P8:595:SER:C       | 5:P8:597:GLY:H      | 1.55                     | 1.11              |
| 5:P16:57:PRO:HB2     | 6:O16:29:LEU:HD12   | 1.26                     | 1.11              |
| 8:L8:1041:SER:CB     | 8:L8:1054:HIS:CE1   | 2.33                     | 1.11              |
| 8:L16:1071:LEU:HD21  | 9:K16:1284:MET:SD   | 1.89                     | 1.11              |
| 9:K:584:SER:OG       | 9:K:622:VAL:HG21    | 1.49                     | 1.11              |
| 9:K8:1153:ALA:O      | 9:K8:1220:ASN:CG    | 1.93                     | 1.11              |
| 10:C16:627:VAL:HG12  | 10:C16:628:GLY:H    | 1.11                     | 1.11              |
| 10:C24:565:ARG:HD2   | 10:C24:568:TRP:CE3  | 1.85                     | 1.11              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:453:LEU:HD23   | 10:C:459:LEU:HD11   | 1.17                     | 1.11              |
| 22:I8:199:PHE:CB    | 23:J8:620:MET:SD    | 2.38                     | 1.11              |
| 21:H24:291:VAL:HG12 | 23:J24:657:GLU:HG2  | 1.17                     | 1.11              |
| 21:H24:322:LEU:CB   | 22:I24:300:LEU:HD11 | 1.79                     | 1.11              |
| 10:C32:667:ILE:CD1  | 10:C32:700:MET:HE2  | 1.81                     | 1.11              |
| 2:M:627:TYR:HE2     | 3:N:166:ALA:N       | 1.42                     | 1.11              |
| 1:R16:1187:ARG:HH22 | 1:R16:1201:LEU:HD11 | 0.97                     | 1.11              |
| 2:M16:851:LEU:HD21  | 4:T16:653:GLN:HG2   | 1.32                     | 1.11              |
| 5:P8:105:ARG:NH2    | 5:P8:130:VAL:HA     | 1.62                     | 1.11              |
| 6:O16:82:LEU:HD23   | 6:O16:103:MET:CE    | 1.78                     | 1.11              |
| 8:L8:1077:LEU:HD13  | 9:K8:1086:VAL:HG12  | 1.25                     | 1.11              |
| 10:C24:323:HIS:CE1  | 10:C24:327:ILE:HD11 | 1.85                     | 1.11              |
| 10:C24:1050:HIS:CD2 | 10:C24:1086:LYS:NZ  | 2.19                     | 1.11              |
| 11:A32:91:GLU:HB3   | 18:B8:1112:LYS:HE2  | 1.11                     | 1.11              |
| 20:E:353:ILE:HG21   | 20:E:413:PHE:CE2    | 1.84                     | 1.11              |
| 23:J8:718:GLN:NE2   | 23:J8:737:TRP:HZ3   | 1.32                     | 1.11              |
| 12:A48:707:LEU:HG   | 12:A48:767:ARG:NH2  | 1.66                     | 1.11              |
| 1:R:1078:SER:HB2    | 5:P:713:LEU:HD21    | 1.32                     | 1.10              |
| 2:M:345:ASP:O       | 2:M:347:LYS:N       | 1.84                     | 1.10              |
| 5:P8:57:PRO:HB2     | 6:O8:29:LEU:HD11    | 1.20                     | 1.10              |
| 9:K:1085:TYR:OH     | 9:K:1093:SER:CA     | 1.99                     | 1.10              |
| 9:K:1153:ALA:O      | 9:K:1220:ASN:CG     | 1.93                     | 1.10              |
| 9:K8:975:MET:HE3    | 9:K8:989:VAL:HG11   | 1.23                     | 1.10              |
| 10:C16:1050:HIS:CD2 | 10:C16:1086:LYS:NZ  | 2.19                     | 1.10              |
| 10:C24:499:LEU:HD23 | 10:C24:505:PHE:CE2  | 1.86                     | 1.10              |
| 11:A40:156:MET:HA   | 11:A40:555:HIS:CD2  | 1.87                     | 1.10              |
| 10:C:452:LEU:HD11   | 10:C:453:LEU:HG     | 1.23                     | 1.10              |
| 10:C:1050:HIS:CD2   | 10:C:1086:LYS:NZ    | 2.19                     | 1.10              |
| 18:B8:536:ILE:HG23  | 18:B8:545:VAL:CG1   | 1.80                     | 1.10              |
| 24:D:409:LEU:CD1    | 24:D16:746:ALA:N    | 2.13                     | 1.10              |
| 7:Q8:143:ARG:NH2    | 7:Q8:147:GLU:OE2    | 1.83                     | 1.10              |
| 5:P16:112:LEU:CD2   | 5:P16:122:TYR:CG    | 2.34                     | 1.10              |
| 8:L16:1069:LEU:HD11 | 9:K16:1086:VAL:HG11 | 1.29                     | 1.10              |
| 9:K8:584:SER:OG     | 9:K8:622:VAL:HG21   | 1.49                     | 1.10              |
| 10:C16:499:LEU:HD23 | 10:C16:505:PHE:HE2  | 1.08                     | 1.10              |
| 12:A:440:LEU:CB     | 12:A:443:LEU:CD1    | 2.29                     | 1.10              |
| 10:C8:1050:HIS:CD2  | 10:C8:1086:LYS:NZ   | 2.19                     | 1.10              |
| 11:A16:440:LEU:CB   | 11:A16:443:LEU:CD1  | 2.29                     | 1.10              |
| 11:A32:440:LEU:HB2  | 11:A32:443:LEU:HD12 | 1.24                     | 1.10              |
| 19:4:180:ALA:HB3    | 19:4:202:ILE:HD11   | 1.21                     | 1.10              |
| 21:H8:363:MET:SD    | 22:I8:332:MET:HE1   | 1.90                     | 1.10              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:J16:718:GLN:NE2  | 23:J16:737:TRP:HZ3  | 1.32                     | 1.10              |
| 24:D:1385:MET:SD    | 24:D:1464:PHE:CE1   | 2.44                     | 1.10              |
| 3:N:162:THR:HG23    | 3:N:168:VAL:HG22    | 1.29                     | 1.10              |
| 3:N8:4:GLN:HE22     | 3:N8:44:GLY:HA2     | 1.11                     | 1.10              |
| 2:M16:185:ARG:HH11  | 2:M16:213:LEU:CD1   | 1.63                     | 1.10              |
| 2:M16:672:TYR:CD2   | 2:M16:680:LYS:HD3   | 1.87                     | 1.10              |
| 5:P:401:ARG:HG2     | 5:P:414:VAL:HG11    | 1.28                     | 1.10              |
| 5:P:402:LEU:HD13    | 5:P:433:LEU:CB      | 1.82                     | 1.10              |
| 5:P16:101:LEU:HD22  | 5:P16:133:TYR:OH    | 1.46                     | 1.10              |
| 9:K:634:LEU:HD22    | 9:K:754:ARG:HH12    | 1.12                     | 1.10              |
| 10:C16:1271:PHE:CZ  | 10:C16:1284:ASP:CG  | 2.30                     | 1.10              |
| 11:A40:707:LEU:HG   | 11:A40:767:ARG:NH2  | 1.66                     | 1.10              |
| 13:V:787:ILE:CD1    | 15:J:592:VAL:HG13   | 1.82                     | 1.10              |
| 10:C:565:ARG:NH2    | 10:C:569:PHE:CD2    | 2.20                     | 1.10              |
| 11:A16:137:GLU:HG3  | 18:B:1901:GLN:NE2   | 1.64                     | 1.10              |
| 19:4:250:ILE:HD13   | 20:E:165:ARG:HH21   | 1.14                     | 1.10              |
| 20:E:352:PHE:CE1    | 20:E:451:ILE:CD1    | 2.33                     | 1.10              |
| 19:48:180:ALA:HB3   | 19:48:202:ILE:HD11  | 1.21                     | 1.10              |
| 21:H24:231:HIS:CD2  | 23:J24:596:GLN:HE21 | 1.57                     | 1.10              |
| 22:I16:199:PHE:CB   | 23:J16:620:MET:SD   | 2.38                     | 1.10              |
| 10:C32:499:LEU:HD23 | 10:C32:505:PHE:CE2  | 1.86                     | 1.10              |
| 1:R:1324:ASP:CG     | 10:C:1180:ILE:CG2   | 2.25                     | 1.10              |
| 2:M:185:ARG:HH11    | 2:M:213:LEU:CD1     | 1.64                     | 1.10              |
| 2:M:416:VAL:HG11    | 8:L:398:ALA:HB2     | 1.11                     | 1.10              |
| 2:M8:345:ASP:O      | 2:M8:347:LYS:N      | 1.84                     | 1.10              |
| 10:C16:557:VAL:HG22 | 10:C16:565:ARG:NH2  | 1.65                     | 1.10              |
| 10:C24:110:ARG:HH11 | 10:C24:118:LEU:CD1  | 1.65                     | 1.10              |
| 10:C24:1271:PHE:CZ  | 10:C24:1284:ASP:CG  | 2.30                     | 1.10              |
| 18:B:536:ILE:HG23   | 18:B:545:VAL:CG1    | 1.80                     | 1.10              |
| 18:B8:154:LEU:HD21  | 18:B8:224:GLU:HG3   | 1.29                     | 1.10              |
| 18:B8:789:LEU:HD23  | 18:B8:793:LEU:HD12  | 1.30                     | 1.10              |
| 18:B8:1130:LEU:HD23 | 18:B8:1132:TRP:HE1  | 1.11                     | 1.10              |
| 24:D:409:LEU:CD1    | 24:D16:746:ALA:CA   | 2.19                     | 1.10              |
| 10:C32:453:LEU:HD23 | 10:C32:459:LEU:HD11 | 1.18                     | 1.10              |
| 10:C32:667:ILE:HD12 | 10:C32:700:MET:HE2  | 1.28                     | 1.10              |
| 10:C32:1271:PHE:CZ  | 10:C32:1284:ASP:CG  | 2.30                     | 1.10              |
| 1:R:1022:TYR:HE1    | 24:D:1441:PRO:HG3   | 1.17                     | 1.10              |
| 1:R:1425:PRO:CA     | 6:O:165:LYS:NZ      | 2.14                     | 1.10              |
| 5:P:175:MET:HE1     | 5:P:436:ALA:HB1     | 1.34                     | 1.10              |
| 10:C16:565:ARG:HD2  | 10:C16:568:TRP:CE3  | 1.86                     | 1.10              |
| 10:C24:345:MET:HE3  | 10:C24:401:ILE:CD1  | 1.80                     | 1.10              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:W:586:ILE:HD12   | 15:J:569:ALA:HA     | 1.21                     | 1.10              |
| 10:C8:499:LEU:HD23  | 10:C8:505:PHE:CE2   | 1.86                     | 1.10              |
| 10:C8:1265:ARG:O    | 10:C8:1268:ARG:HG2  | 1.35                     | 1.10              |
| 11:A32:440:LEU:CB   | 11:A32:443:LEU:CD1  | 2.28                     | 1.10              |
| 18:B8:1130:LEU:HD23 | 18:B8:1132:TRP:NE1  | 1.65                     | 1.10              |
| 18:B8:1205:ILE:HD11 | 18:B8:1271:PHE:CD2  | 1.86                     | 1.10              |
| 19:48:4:PHE:CE2     | 19:48:378:TYR:CE1   | 2.40                     | 1.10              |
| 22:I16:300:LEU:CD2  | 23:J16:689:LEU:HD21 | 1.82                     | 1.10              |
| 10:C32:1050:HIS:CD2 | 10:C32:1086:LYS:NZ  | 2.18                     | 1.10              |
| 1:R:1434:VAL:HG13   | 2:M:176:VAL:HG22    | 1.24                     | 1.09              |
| 1:R16:1434:VAL:HG13 | 2:M16:176:VAL:HG22  | 1.24                     | 1.09              |
| 5:P:175:MET:HE1     | 5:P:436:ALA:CB      | 1.82                     | 1.09              |
| 7:Q:143:ARG:NH2     | 7:Q:147:GLU:OE2     | 1.84                     | 1.09              |
| 10:C:643:LEU:CD1    | 10:C:679:ARG:HH11   | 1.65                     | 1.09              |
| 10:C:679:ARG:HH22   | 10:C:690:LEU:HD21   | 0.93                     | 1.09              |
| 10:C:1271:PHE:CZ    | 10:C:1284:ASP:CG    | 2.30                     | 1.09              |
| 10:C8:1163:LEU:HD23 | 10:C8:1166:SER:OG   | 1.48                     | 1.09              |
| 11:A16:676:TYR:CE2  | 24:D16:1395:SER:CA  | 2.35                     | 1.09              |
| 18:B:536:ILE:HG23   | 18:B:545:VAL:HG11   | 1.32                     | 1.09              |
| 18:B:1725:THR:HG23  | 18:B:1830:LEU:HD22  | 1.34                     | 1.09              |
| 10:C32:667:ILE:O    | 10:C32:668:ALA:C    | 1.68                     | 1.09              |
| 10:C32:768:ARG:NH2  | 10:C32:775:LYS:HG2  | 1.67                     | 1.09              |
| 1:R:771:SER:HB2     | 24:D:1317:ARG:HD2   | 1.34                     | 1.09              |
| 3:N:43:ASN:ND2      | 10:C:503:THR:HG21   | 1.66                     | 1.09              |
| 3:N:162:THR:HG21    | 3:N:168:VAL:HG23    | 1.14                     | 1.09              |
| 2:M8:417:ARG:CB     | 8:L8:298:PHE:CE2    | 2.19                     | 1.09              |
| 2:M8:626:PRO:CD     | 3:N8:165:GLY:O      | 2.00                     | 1.09              |
| 1:R16:1460:MET:CE   | 1:R16:1463:GLN:OE1  | 2.01                     | 1.09              |
| 8:L:605:MET:SD      | 8:L:631:LEU:CD1     | 2.40                     | 1.09              |
| 8:L8:976:LEU:HD22   | 9:K8:1004:ARG:CD    | 1.69                     | 1.09              |
| 8:L16:1069:LEU:HD11 | 9:K16:1086:VAL:CG1  | 1.82                     | 1.09              |
| 10:C16:62:ILE:HD12  | 10:C16:72:LEU:HD11  | 1.31                     | 1.09              |
| 12:A:642:GLY:HA3    | 12:A:685:ARG:NH1    | 1.67                     | 1.09              |
| 14:W:659:ARG:HH22   | 15:J:583:LEU:HD23   | 1.04                     | 1.09              |
| 10:C:499:LEU:HD23   | 10:C:505:PHE:HE2    | 1.08                     | 1.09              |
| 18:B:86:LYS:HG2     | 18:B:123:LEU:CD1    | 1.82                     | 1.09              |
| 18:B:428:GLN:HG3    | 18:B:584:ARG:HH12   | 1.13                     | 1.09              |
| 18:B8:428:GLN:HG3   | 18:B8:584:ARG:HH12  | 1.13                     | 1.09              |
| 22:I:300:LEU:CD2    | 23:J32:689:LEU:HD21 | 1.82                     | 1.09              |
| 24:D8:1330:ARG:NH1  | 24:D16:719:ARG:HB2  | 1.68                     | 1.09              |
| 10:C32:345:MET:HE3  | 10:C32:401:ILE:CD1  | 1.80                     | 1.09              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R:1022:TYR:OH      | 24:D:1441:PRO:HB3    | 1.52                     | 1.09              |
| 2:M8:185:ARG:HH11    | 2:M8:213:LEU:CD1     | 1.64                     | 1.09              |
| 2:M16:626:PRO:CD     | 3:N16:165:GLY:O      | 2.00                     | 1.09              |
| 5:P8:611:LEU:HA      | 5:P8:629:ARG:NE      | 1.67                     | 1.09              |
| 8:L:1081:MET:SD      | 9:K:1083:ILE:HG21    | 1.89                     | 1.09              |
| 9:K:578:THR:HG21     | 9:K:616:ARG:NH2      | 1.67                     | 1.09              |
| 9:K:1074:ARG:HD2     | 9:K:1126:LEU:HD21    | 1.33                     | 1.09              |
| 9:K8:1085:TYR:OH     | 9:K8:1093:SER:CA     | 1.99                     | 1.09              |
| 10:C16:1050:HIS:CD2  | 10:C16:1086:LYS:HZ2  | 1.69                     | 1.09              |
| 11:A24:737:GLU:HG3   | 24:D16:871:ARG:NH2   | 1.67                     | 1.09              |
| 10:C24:110:ARG:NH1   | 10:C24:118:LEU:CD1   | 2.16                     | 1.09              |
| 10:C24:345:MET:HE1   | 10:C24:401:ILE:HD12  | 1.26                     | 1.09              |
| 10:C24:1703:ILE:HD12 | 10:C24:1741:MET:HE1  | 1.29                     | 1.09              |
| 11:A40:390:ALA:HB1   | 24:D32:1099:ARG:HD2  | 1.35                     | 1.09              |
| 14:W:1:MET:HE2       | 10:C:1497:LYS:HD3    | 1.24                     | 1.09              |
| 10:C:452:LEU:CD1     | 10:C:453:LEU:HG      | 1.80                     | 1.09              |
| 10:C:1163:LEU:HD23   | 10:C:1166:SER:OG     | 1.48                     | 1.09              |
| 10:C8:667:ILE:HD13   | 10:C8:697:HIS:ND1    | 1.67                     | 1.09              |
| 10:C8:1271:PHE:CZ    | 10:C8:1284:ASP:CG    | 2.30                     | 1.09              |
| 19:4:250:ILE:HD11    | 20:E:163:ILE:HD13    | 1.34                     | 1.09              |
| 23:J32:686:MET:CE    | 23:J32:694:ARG:NH2   | 2.16                     | 1.09              |
| 10:C32:1466:ARG:HA   | 10:C32:1469:HIS:CE1  | 1.88                     | 1.09              |
| 1:R:1326:GLY:HA3     | 10:C:1154:TRP:HE1    | 1.06                     | 1.09              |
| 2:M:844:VAL:HG22     | 4:T:660:LEU:HD21     | 1.14                     | 1.09              |
| 1:R8:526:ASN:HA      | 1:R8:529:HIS:CE1     | 1.88                     | 1.09              |
| 2:M16:345:ASP:O      | 2:M16:347:LYS:N      | 1.85                     | 1.09              |
| 5:P:633:LEU:HD22     | 5:P:647:LEU:HD13     | 1.22                     | 1.09              |
| 10:C16:768:ARG:NH2   | 10:C16:775:LYS:HG2   | 1.67                     | 1.09              |
| 14:W:516:GLN:HA      | 14:W:604:PRO:O       | 0.92                     | 1.09              |
| 10:C:1285:VAL:HG23   | 10:C:1738:MET:CE     | 1.83                     | 1.09              |
| 10:C8:110:ARG:HH11   | 10:C8:118:LEU:CD1    | 1.65                     | 1.09              |
| 10:C8:345:MET:HE1    | 10:C8:401:ILE:HD12   | 1.26                     | 1.09              |
| 10:C8:453:LEU:HD23   | 10:C8:459:LEU:HD11   | 1.18                     | 1.09              |
| 10:C8:768:ARG:CZ     | 10:C8:775:LYS:HG2    | 1.82                     | 1.09              |
| 10:C8:960:PHE:CZ     | 10:C8:1138:GLU:CG    | 2.35                     | 1.09              |
| 10:C8:1703:ILE:HD12  | 10:C8:1741:MET:HE1   | 1.29                     | 1.09              |
| 11:A16:707:LEU:HG    | 11:A16:767:ARG:NH2   | 1.66                     | 1.09              |
| 18:B:1529:GLU:CD     | 24:D16:1415:LEU:HD11 | 1.76                     | 1.09              |
| 21:H16:363:MET:SD    | 22:I16:332:MET:HE1   | 1.90                     | 1.09              |
| 24:D32:749:ARG:HH12  | 24:D40:396:GLY:HA2   | 1.12                     | 1.09              |
| 10:C32:572:ILE:CD1   | 10:C32:606:MET:CE    | 2.24                     | 1.09              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 3:N:19:MET:HE2       | 3:N:23:GLY:CA        | 1.83                     | 1.09              |
| 2:M8:672:TYR:HB2     | 2:M8:680:LYS:HD3     | 1.15                     | 1.09              |
| 1:R16:526:ASN:HA     | 1:R16:529:HIS:CE1    | 1.88                     | 1.09              |
| 3:N16:19:MET:HE2     | 3:N16:23:GLY:CA      | 1.83                     | 1.09              |
| 5:P:402:LEU:HD22     | 5:P:433:LEU:HD13     | 1.34                     | 1.09              |
| 8:L:1069:LEU:HD11    | 9:K:1086:VAL:HG11    | 1.16                     | 1.09              |
| 8:L8:1074:ARG:HD3    | 9:K8:1089:LYS:HG2    | 1.21                     | 1.09              |
| 8:L16:605:MET:SD     | 8:L16:631:LEU:CD1    | 2.40                     | 1.09              |
| 10:C16:110:ARG:NH1   | 10:C16:118:LEU:CD1   | 2.16                     | 1.09              |
| 10:C16:499:LEU:HD23  | 10:C16:505:PHE:CE2   | 1.86                     | 1.09              |
| 10:C16:565:ARG:NH2   | 10:C16:569:PHE:CD2   | 2.20                     | 1.09              |
| 10:C16:1703:ILE:HD12 | 10:C16:1741:MET:HE1  | 1.29                     | 1.09              |
| 10:C24:565:ARG:HD3   | 10:C24:568:TRP:CE3   | 1.84                     | 1.09              |
| 10:C24:847:ARG:NH2   | 10:C24:903:ASN:HB3   | 1.67                     | 1.09              |
| 11:A40:390:ALA:CB    | 24:D32:1099:ARG:HB2  | 1.81                     | 1.09              |
| 10:C:847:ARG:NH2     | 10:C:903:ASN:HB3     | 1.67                     | 1.09              |
| 11:A16:90:PHE:CE1    | 18:B:1788:ILE:CG2    | 2.36                     | 1.09              |
| 11:A32:676:TYR:CE2   | 24:D32:1395:SER:HB2  | 1.73                     | 1.09              |
| 11:A32:703:ALA:HB1   | 24:D32:1398:ARG:HH11 | 1.16                     | 1.09              |
| 18:B:1110:LEU:HD13   | 21:H:323:TYR:OH      | 1.25                     | 1.09              |
| 18:B8:1725:THR:HG23  | 18:B8:1830:LEU:HD22  | 1.34                     | 1.09              |
| 22:I24:300:LEU:CD2   | 23:J24:689:LEU:HD21  | 1.82                     | 1.09              |
| 23:J24:686:MET:CE    | 23:J24:694:ARG:NH2   | 2.16                     | 1.09              |
| 12:A48:440:LEU:HB2   | 12:A48:443:LEU:HD12  | 1.24                     | 1.09              |
| 8:L16:1069:LEU:HD21  | 9:K16:1086:VAL:HG11  | 1.33                     | 1.08              |
| 12:A:519:MET:HE1     | 12:A:569:MET:HE3     | 1.15                     | 1.08              |
| 10:C:110:ARG:NH1     | 10:C:118:LEU:CD1     | 2.16                     | 1.08              |
| 10:C:557:VAL:HG22    | 10:C:565:ARG:NH2     | 1.67                     | 1.08              |
| 11:A16:91:GLU:N      | 18:B:1800:ARG:HH22   | 1.51                     | 1.08              |
| 11:A32:560:MET:HE1   | 11:A32:615:GLN:HE22  | 1.05                     | 1.08              |
| 18:B:789:LEU:HD23    | 18:B:793:LEU:HD12    | 1.30                     | 1.08              |
| 18:B8:786:ASP:OD2    | 24:D32:1066:VAL:CB   | 2.01                     | 1.08              |
| 24:D40:873:ARG:HH11  | 24:D40:884:ASP:CB    | 1.64                     | 1.08              |
| 10:C32:345:MET:CE    | 10:C32:401:ILE:HD13  | 1.75                     | 1.08              |
| 10:C32:627:VAL:HG12  | 10:C32:628:GLY:H     | 1.11                     | 1.08              |
| 10:C32:643:LEU:CD1   | 10:C32:679:ARG:HH11  | 1.65                     | 1.08              |
| 12:A48:519:MET:CE    | 12:A48:569:MET:CE    | 2.31                     | 1.08              |
| 1:R:1175:TYR:HA      | 1:R:1177:TRP:CZ3     | 1.87                     | 1.08              |
| 1:R:1326:GLY:CA      | 10:C:1154:TRP:HE1    | 1.65                     | 1.08              |
| 1:R8:1460:MET:CE     | 1:R8:1463:GLN:OE1    | 2.01                     | 1.08              |
| 11:A24:440:LEU:CB    | 11:A24:443:LEU:CD1   | 2.29                     | 1.08              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A24:468:VAL:HG21  | 24:D16:1100:GLN:OE1  | 1.54                     | 1.08              |
| 11:A40:468:VAL:HG21  | 24:D32:1100:GLN:OE1  | 1.53                     | 1.08              |
| 10:C:345:MET:HE1     | 10:C:401:ILE:HD12    | 1.26                     | 1.08              |
| 10:C8:847:ARG:NH2    | 10:C8:903:ASN:HB3    | 1.67                     | 1.08              |
| 11:A16:52:LEU:HD23   | 11:A16:55:GLU:OE2    | 1.53                     | 1.08              |
| 11:A32:122:LYS:CE    | 18:B8:1757:GLU:OE1   | 2.01                     | 1.08              |
| 18:B:928:ARG:CZ      | 18:B:969:ASP:O       | 2.00                     | 1.08              |
| 18:B:1575:GLN:NE2    | 24:D16:1403:LEU:CD2  | 1.97                     | 1.08              |
| 18:B8:460:PRO:O      | 18:B8:562:ARG:NH1    | 1.86                     | 1.08              |
| 18:B8:1529:GLU:CD    | 24:D32:1415:LEU:HD11 | 1.77                     | 1.08              |
| 19:4:4:PHE:CE2       | 19:4:378:TYR:CE1     | 2.40                     | 1.08              |
| 20:E8:434:TRP:HE1    | 24:D40:72:GLU:CD     | 1.61                     | 1.08              |
| 1:R8:1175:TYR:HA     | 1:R8:1177:TRP:CZ3    | 1.87                     | 1.08              |
| 5:P8:105:ARG:NE      | 5:P8:130:VAL:HG22    | 1.68                     | 1.08              |
| 8:L8:270:LEU:HD23    | 12:A48:155:SER:HB2   | 1.35                     | 1.08              |
| 9:K8:955:TYR:CE1     | 9:K8:985:PHE:HB2     | 1.87                     | 1.08              |
| 10:C16:1285:VAL:HG23 | 10:C16:1738:MET:CE   | 1.82                     | 1.08              |
| 10:C24:1547:LYS:NZ   | 24:D24:1405:GLY:N    | 2.01                     | 1.08              |
| 14:W:516:GLN:CA      | 14:W:604:PRO:C       | 2.22                     | 1.08              |
| 10:C:153:ALA:CB      | 24:D:1403:LEU:CD1    | 2.32                     | 1.08              |
| 10:C:1466:ARG:HA     | 10:C:1469:HIS:CE1    | 1.88                     | 1.08              |
| 11:A16:91:GLU:OE2    | 18:B:1112:LYS:HD3    | 1.45                     | 1.08              |
| 11:A32:519:MET:CE    | 11:A32:569:MET:CE    | 2.31                     | 1.08              |
| 11:A32:707:LEU:HG    | 11:A32:767:ARG:NH2   | 1.66                     | 1.08              |
| 18:B:154:LEU:HD21    | 18:B:224:GLU:HG3     | 1.29                     | 1.08              |
| 18:B8:712:PRO:CG     | 18:B8:759:MET:HE2    | 1.78                     | 1.08              |
| 18:B8:928:ARG:CZ     | 18:B8:969:ASP:O      | 2.00                     | 1.08              |
| 22:I8:300:LEU:CD2    | 23:J8:689:LEU:HD21   | 1.82                     | 1.08              |
| 10:C32:345:MET:HE1   | 10:C32:401:ILE:HD12  | 1.26                     | 1.08              |
| 2:M:363:ARG:NH1      | 2:M:494:SER:O        | 1.87                     | 1.08              |
| 3:N8:162:THR:HG21    | 3:N8:168:VAL:HG23    | 1.14                     | 1.08              |
| 5:P8:57:PRO:HB2      | 6:O8:29:LEU:HD12     | 1.26                     | 1.08              |
| 7:Q16:124:PHE:CE1    | 7:Q16:125:TYR:CZ     | 2.41                     | 1.08              |
| 8:L8:976:LEU:CD2     | 9:K8:1004:ARG:NE     | 2.09                     | 1.08              |
| 10:C16:407:LYS:CE    | 10:C16:465:PHE:CE2   | 2.26                     | 1.08              |
| 10:C16:847:ARG:NH2   | 10:C16:903:ASN:HB3   | 1.67                     | 1.08              |
| 10:C24:407:LYS:HG3   | 10:C24:465:PHE:CZ    | 1.88                     | 1.08              |
| 10:C24:667:ILE:O     | 10:C24:668:ALA:C     | 1.68                     | 1.08              |
| 11:A40:52:LEU:HD23   | 11:A40:55:GLU:OE2    | 1.53                     | 1.08              |
| 11:A40:519:MET:CE    | 11:A40:569:MET:CE    | 2.31                     | 1.08              |
| 10:C8:110:ARG:NH1    | 10:C8:118:LEU:CD1    | 2.16                     | 1.08              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C8:345:MET:HE3   | 10:C8:401:ILE:CD1    | 1.80                     | 1.08              |
| 11:A16:560:MET:HE1  | 11:A16:615:GLN:HE22  | 1.05                     | 1.08              |
| 11:A32:519:MET:HE1  | 11:A32:569:MET:HE3   | 1.15                     | 1.08              |
| 18:B:262:HIS:ND1    | 18:B:379:LEU:HD21    | 1.69                     | 1.08              |
| 10:C32:110:ARG:NH1  | 10:C32:118:LEU:CD1   | 2.16                     | 1.08              |
| 10:C32:407:LYS:HG3  | 10:C32:465:PHE:CZ    | 1.88                     | 1.08              |
| 2:M8:162:ILE:CD1    | 2:M8:213:LEU:HG      | 1.83                     | 1.08              |
| 2:M16:672:TYR:CG    | 2:M16:680:LYS:CD     | 2.37                     | 1.08              |
| 5:P:15:LEU:HD22     | 6:O:309:SER:O        | 1.53                     | 1.08              |
| 10:C16:110:ARG:HH11 | 10:C16:118:LEU:CD1   | 1.65                     | 1.08              |
| 10:C16:407:LYS:HG3  | 10:C16:465:PHE:CZ    | 1.88                     | 1.08              |
| 11:A24:555:HIS:O    | 11:A24:557:LEU:N     | 1.87                     | 1.08              |
| 10:C24:452:LEU:HD13 | 10:C24:452:LEU:O     | 1.51                     | 1.08              |
| 13:V:794:ILE:HD12   | 15:J:599:LEU:CD2     | 1.84                     | 1.08              |
| 14:W:515:CYS:HB3    | 14:W:604:PRO:HD3     | 1.30                     | 1.08              |
| 10:C8:1466:ARG:HA   | 10:C8:1469:HIS:CE1   | 1.88                     | 1.08              |
| 18:B8:86:LYS:HG2    | 18:B8:123:LEU:CD1    | 1.82                     | 1.08              |
| 19:4:189:LEU:HD13   | 19:4:203:LEU:HD23    | 1.28                     | 1.08              |
| 20:E:433:LYS:O      | 20:E:435:ALA:N       | 1.86                     | 1.08              |
| 19:48:188:ALA:O     | 19:48:190:ARG:N      | 1.86                     | 1.08              |
| 20:E8:433:LYS:O     | 20:E8:435:ALA:N      | 1.86                     | 1.08              |
| 21:H16:255:LEU:CD1  | 23:J16:655:GLU:OE2   | 2.02                     | 1.08              |
| 23:J16:686:MET:CE   | 23:J16:694:ARG:NH2   | 2.16                     | 1.08              |
| 10:C32:847:ARG:NH2  | 10:C32:903:ASN:HB3   | 1.67                     | 1.08              |
| 12:A48:806:GLN:OE1  | 12:A48:847:ARG:NH2   | 1.87                     | 1.08              |
| 1:R:526:ASN:HA      | 1:R:529:HIS:CE1      | 1.88                     | 1.07              |
| 1:R:1033:LYS:HZ1    | 24:D:1432:THR:CB     | 1.65                     | 1.07              |
| 2:M:162:ILE:CD1     | 2:M:213:LEU:HG       | 1.83                     | 1.07              |
| 2:M:626:PRO:CD      | 3:N:165:GLY:O        | 2.00                     | 1.07              |
| 2:M16:544:LEU:HD11  | 2:M16:586:ALA:C      | 1.79                     | 1.07              |
| 10:C16:390:HIS:HD2  | 10:C16:452:LEU:CG    | 1.67                     | 1.07              |
| 10:C16:1466:ARG:HA  | 10:C16:1469:HIS:CE1  | 1.88                     | 1.07              |
| 10:C24:228:ARG:NH2  | 10:C24:277:SER:CB    | 2.17                     | 1.07              |
| 10:C24:565:ARG:NH2  | 10:C24:569:PHE:CD2   | 2.20                     | 1.07              |
| 12:A:519:MET:CE     | 12:A:569:MET:CE      | 2.31                     | 1.07              |
| 11:A16:718:THR:HG23 | 24:D16:1398:ARG:HH12 | 1.16                     | 1.07              |
| 11:A32:52:LEU:HD23  | 11:A32:55:GLU:OE2    | 1.53                     | 1.07              |
| 18:B8:783:LYS:HE3   | 24:D32:1064:GLY:HA2  | 1.34                     | 1.07              |
| 22:I:146:SER:HB3    | 23:J32:574:ARG:NH1   | 1.69                     | 1.07              |
| 23:J8:686:MET:CE    | 23:J8:694:ARG:NH2    | 2.16                     | 1.07              |
| 10:C32:667:ILE:HD12 | 10:C32:700:MET:CE    | 1.84                     | 1.07              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C32:668:ALA:HA   | 10:C32:700:MET:HE1  | 1.21                     | 1.07              |
| 2:M:672:TYR:CB      | 2:M:680:LYS:HD2     | 1.84                     | 1.07              |
| 1:R8:1187:ARG:HH22  | 1:R8:1201:LEU:HD11  | 0.97                     | 1.07              |
| 2:M16:162:ILE:CD1   | 2:M16:213:LEU:HG    | 1.83                     | 1.07              |
| 7:Q:187:TRP:HH2     | 7:Q:207:GLN:NE2     | 1.53                     | 1.07              |
| 7:Q8:297:VAL:HG11   | 7:Q8:301:ARG:HB2    | 1.33                     | 1.07              |
| 5:P16:179:TYR:CE1   | 5:P16:436:ALA:C     | 2.22                     | 1.07              |
| 8:L16:1034:VAL:HG21 | 8:L16:1068:PHE:HE2  | 0.91                     | 1.07              |
| 9:K8:1232:LEU:CD2   | 9:K8:1265:ILE:CG2   | 2.29                     | 1.07              |
| 10:C16:228:ARG:NH2  | 10:C16:277:SER:CB   | 2.17                     | 1.07              |
| 10:C24:667:ILE:HD13 | 10:C24:670:GLU:O    | 1.53                     | 1.07              |
| 10:C24:768:ARG:NH2  | 10:C24:775:LYS:HG2  | 1.67                     | 1.07              |
| 11:A40:707:LEU:HG   | 11:A40:767:ARG:HH22 | 1.12                     | 1.07              |
| 12:A:806:GLN:OE1    | 12:A:847:ARG:NH2    | 1.87                     | 1.07              |
| 13:V:790:GLN:HE22   | 14:W:674:GLN:NE2    | 1.38                     | 1.07              |
| 14:W:586:ILE:HD13   | 15:J:569:ALA:HA     | 1.30                     | 1.07              |
| 10:C:110:ARG:HH11   | 10:C:118:LEU:CD1    | 1.65                     | 1.07              |
| 10:C:345:MET:HE3    | 10:C:401:ILE:CD1    | 1.80                     | 1.07              |
| 10:C:557:VAL:HG22   | 10:C:565:ARG:HH21   | 0.95                     | 1.07              |
| 11:A16:519:MET:CE   | 11:A16:569:MET:CE   | 2.31                     | 1.07              |
| 11:A16:707:LEU:HG   | 11:A16:767:ARG:HH22 | 1.12                     | 1.07              |
| 11:A32:707:LEU:HG   | 11:A32:767:ARG:HH22 | 1.12                     | 1.07              |
| 18:B:154:LEU:HD21   | 18:B:224:GLU:CG     | 1.84                     | 1.07              |
| 18:B:428:GLN:HG3    | 18:B:584:ARG:NH1    | 1.69                     | 1.07              |
| 18:B:1273:GLU:CG    | 18:B:1276:LYS:HE3   | 1.84                     | 1.07              |
| 19:4:188:ALA:O      | 19:4:190:ARG:N      | 1.86                     | 1.07              |
| 22:I24:146:SER:HB3  | 23:J24:574:ARG:HH12 | 0.92                     | 1.07              |
| 21:H16:291:VAL:HG12 | 23:J16:657:GLU:HG2  | 1.17                     | 1.07              |
| 1:R:1460:MET:CE     | 1:R:1463:GLN:OE1    | 2.01                     | 1.07              |
| 7:Q8:124:PHE:CE1    | 7:Q8:125:TYR:CZ     | 2.41                     | 1.07              |
| 7:Q16:187:TRP:HH2   | 7:Q16:207:GLN:NE2   | 1.53                     | 1.07              |
| 9:K8:578:THR:HG21   | 9:K8:616:ARG:NH2    | 1.67                     | 1.07              |
| 9:K8:1180:TRP:CD1   | 9:K8:1261:MET:HE2   | 1.89                     | 1.07              |
| 11:A24:52:LEU:HD23  | 11:A24:55:GLU:OE2   | 1.53                     | 1.07              |
| 10:C24:667:ILE:HD13 | 10:C24:697:HIS:HE1  | 1.09                     | 1.07              |
| 14:W:659:ARG:NH2    | 15:J:586:GLU:OE2    | 1.85                     | 1.07              |
| 10:C:228:ARG:NH2    | 10:C:277:SER:CB     | 2.17                     | 1.07              |
| 10:C:848:CYS:HA     | 10:C:906:ARG:HH22   | 1.09                     | 1.07              |
| 11:A16:122:LYS:CE   | 18:B:1757:GLU:OE1   | 2.01                     | 1.07              |
| 11:A16:676:TYR:CE2  | 24:D16:1395:SER:HB2 | 1.89                     | 1.07              |
| 18:B:460:PRO:O      | 18:B:562:ARG:NH1    | 1.86                     | 1.07              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B8:154:LEU:HD21  | 18:B8:224:GLU:CG    | 1.84                     | 1.07              |
| 18:B8:1110:LEU:HD23 | 21:H24:326:GLY:HA2  | 1.23                     | 1.07              |
| 20:E8:353:ILE:CD1   | 20:E8:413:PHE:CG    | 2.37                     | 1.07              |
| 24:D8:1330:ARG:HH12 | 24:D16:719:ARG:HB2  | 1.12                     | 1.07              |
| 1:R:768:LEU:HG      | 24:D:1362:VAL:C     | 1.79                     | 1.07              |
| 1:R:1033:LYS:NZ     | 24:D:1432:THR:CB    | 2.17                     | 1.07              |
| 2:M:628:LEU:HD13    | 3:N:223:GLY:C       | 1.80                     | 1.07              |
| 1:R8:1059:ILE:HG21  | 24:D40:1435:ARG:CZ  | 1.83                     | 1.07              |
| 1:R16:1175:TYR:HA   | 1:R16:1177:TRP:CZ3  | 1.87                     | 1.07              |
| 9:K8:919:MET:SD     | 9:K8:923:ILE:HD12   | 1.94                     | 1.07              |
| 11:A24:362:ARG:CD   | 11:A24:366:ARG:NH2  | 2.18                     | 1.07              |
| 11:A24:560:MET:HE1  | 11:A24:615:GLN:HE22 | 1.05                     | 1.07              |
| 10:C24:1466:ARG:HA  | 10:C24:1469:HIS:CE1 | 1.88                     | 1.07              |
| 10:C8:228:ARG:NH2   | 10:C8:277:SER:CB    | 2.17                     | 1.07              |
| 10:C8:768:ARG:NH2   | 10:C8:775:LYS:HG2   | 1.67                     | 1.07              |
| 11:A16:137:GLU:HG3  | 18:B:1901:GLN:HE22  | 0.90                     | 1.07              |
| 11:A16:806:GLN:OE1  | 11:A16:847:ARG:NH2  | 1.87                     | 1.07              |
| 18:B:1110:LEU:HD23  | 21:H:326:GLY:HA2    | 1.15                     | 1.07              |
| 18:B:1273:GLU:HG2   | 18:B:1276:LYS:CE    | 1.83                     | 1.07              |
| 20:E:235:HIS:NE2    | 20:E:239:LYS:HE3    | 1.70                     | 1.07              |
| 19:48:100:ILE:HG22  | 19:48:102:LEU:HG    | 1.10                     | 1.07              |
| 20:E8:432:ILE:HD13  | 24:D40:72:GLU:CD    | 1.78                     | 1.07              |
| 24:D:400:VAL:HG11   | 24:D16:751:MET:HB2  | 1.09                     | 1.07              |
| 24:D40:839:GLU:HB3  | 24:D40:971:HIS:ND1  | 1.69                     | 1.07              |
| 10:C32:110:ARG:HH11 | 10:C32:118:LEU:CD1  | 1.65                     | 1.07              |
| 10:C32:228:ARG:NH2  | 10:C32:277:SER:CB   | 2.17                     | 1.07              |
| 2:M:417:ARG:HB3     | 8:L:346:TRP:CZ2     | 1.90                     | 1.07              |
| 2:M:851:LEU:HD21    | 4:T:653:GLN:HG2     | 1.32                     | 1.07              |
| 3:N8:19:MET:HE2     | 3:N8:23:GLY:CA      | 1.83                     | 1.07              |
| 5:P:57:PRO:HB2      | 6:O:29:LEU:HD12     | 1.26                     | 1.07              |
| 8:L16:856:LEU:HD23  | 9:K16:1281:SER:CB   | 1.85                     | 1.07              |
| 8:L16:945:ASN:O     | 9:K16:1282:SER:HB2  | 1.55                     | 1.07              |
| 9:K:1154:TRP:CH2    | 9:K:1219:VAL:CG1    | 2.38                     | 1.07              |
| 10:C:768:ARG:NH2    | 10:C:775:LYS:HG2    | 1.67                     | 1.07              |
| 11:A32:806:GLN:OE1  | 11:A32:847:ARG:NH2  | 1.87                     | 1.07              |
| 18:B8:1342:LEU:HD23 | 18:B8:1406:ALA:HB1  | 1.32                     | 1.07              |
| 19:4:100:ILE:HG22   | 19:4:102:LEU:HG     | 1.10                     | 1.07              |
| 19:4:187:SER:O      | 19:4:189:LEU:N      | 1.87                     | 1.07              |
| 12:A48:519:MET:HE1  | 12:A48:569:MET:HE3  | 1.15                     | 1.07              |
| 1:R:1330:ALA:HB3    | 10:C:1173:LEU:HD11  | 1.34                     | 1.06              |
| 2:M:844:VAL:HG21    | 4:T:660:LEU:HD21    | 1.10                     | 1.06              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:417:ARG:CD    | 8:L16:298:PHE:CD2    | 2.21                     | 1.06              |
| 5:P:152:ILE:HD13    | 14:W:762:GLN:HE22    | 0.98                     | 1.06              |
| 5:P8:214:LEU:HD23   | 5:P8:236:VAL:CG1     | 1.85                     | 1.06              |
| 7:Q8:187:TRP:HH2    | 7:Q8:207:GLN:NE2     | 1.53                     | 1.06              |
| 7:Q16:297:VAL:HG11  | 7:Q16:301:ARG:HB2    | 1.33                     | 1.06              |
| 9:K8:840:TRP:CZ3    | 9:K8:907:ILE:CD1     | 2.34                     | 1.06              |
| 10:C24:557:VAL:HG22 | 10:C24:565:ARG:HH21  | 0.93                     | 1.06              |
| 11:A40:555:HIS:O    | 11:A40:557:LEU:N     | 1.87                     | 1.06              |
| 11:A40:691:ALA:HB1  | 24:D24:1397:THR:HG21 | 1.33                     | 1.06              |
| 11:A40:806:GLN:OE1  | 11:A40:847:ARG:NH2   | 1.87                     | 1.06              |
| 10:C8:960:PHE:CE2   | 10:C8:1138:GLU:CG    | 2.37                     | 1.06              |
| 11:A32:362:ARG:CD   | 11:A32:366:ARG:NH2   | 2.18                     | 1.06              |
| 18:B:66:ASN:OD1     | 18:B:84:LYS:NZ       | 1.87                     | 1.06              |
| 18:B:1130:LEU:HD23  | 18:B:1132:TRP:HE1    | 1.11                     | 1.06              |
| 18:B:1940:ALA:CB    | 18:B:1950:ILE:HD11   | 1.85                     | 1.06              |
| 18:B8:1112:LYS:HE3  | 21:H24:327:SER:C     | 1.79                     | 1.06              |
| 18:B8:1273:GLU:HG2  | 18:B8:1276:LYS:CE    | 1.83                     | 1.06              |
| 18:B8:1439:LYS:CE   | 24:D32:1257:ASN:CB   | 2.17                     | 1.06              |
| 21:H24:255:LEU:CD1  | 23:J24:655:GLU:OE2   | 2.02                     | 1.06              |
| 22:I24:146:SER:HB3  | 23:J24:574:ARG:NH1   | 1.69                     | 1.06              |
| 23:J24:718:GLN:CD   | 23:J24:737:TRP:CZ3   | 2.33                     | 1.06              |
| 23:J16:718:GLN:CD   | 23:J16:737:TRP:CZ3   | 2.33                     | 1.06              |
| 4:T:672:GLN:HG3     | 5:P:702:LEU:HD21     | 1.37                     | 1.06              |
| 5:P16:214:LEU:HD23  | 5:P16:236:VAL:CG1    | 1.85                     | 1.06              |
| 10:C16:345:MET:HE3  | 10:C16:401:ILE:CD1   | 1.80                     | 1.06              |
| 10:C24:667:ILE:HG23 | 10:C24:669:GLY:C     | 1.80                     | 1.06              |
| 11:A40:160:THR:C    | 11:A40:491:PRO:HG2   | 1.80                     | 1.06              |
| 10:C8:64:LEU:HD22   | 10:C8:96:ARG:HG3     | 1.38                     | 1.06              |
| 10:C8:847:ARG:HD2   | 10:C8:911:ILE:HD13   | 1.38                     | 1.06              |
| 11:A16:91:GLU:CD    | 18:B:1112:LYS:HD3    | 1.78                     | 1.06              |
| 11:A16:555:HIS:O    | 11:A16:557:LEU:N     | 1.87                     | 1.06              |
| 11:A32:718:THR:HG23 | 24:D32:1398:ARG:HH12 | 1.15                     | 1.06              |
| 18:B:235:ARG:NH1    | 18:B:308:GLU:OE2     | 1.89                     | 1.06              |
| 18:B8:428:GLN:HG3   | 18:B8:584:ARG:NH1    | 1.69                     | 1.06              |
| 18:B8:1273:GLU:CG   | 18:B8:1276:LYS:HE3   | 1.84                     | 1.06              |
| 20:E:353:ILE:CD1    | 20:E:413:PHE:CG      | 2.37                     | 1.06              |
| 19:48:250:ILE:HD13  | 20:E8:165:ARG:HH21   | 1.14                     | 1.06              |
| 21:H:255:LEU:CD1    | 23:J32:655:GLU:OE2   | 2.02                     | 1.06              |
| 24:D:400:VAL:CG1    | 24:D16:751:MET:HB2   | 1.85                     | 1.06              |
| 24:D32:749:ARG:NH1  | 24:D40:396:GLY:HA2   | 1.68                     | 1.06              |
| 10:C32:453:LEU:HD23 | 10:C32:459:LEU:CD1   | 1.86                     | 1.06              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M16:537:ILE:HG13   | 2:M16:558:MET:HE3   | 1.33                     | 1.06              |
| 2:M16:844:VAL:HG22   | 4:T16:660:LEU:HD21  | 1.07                     | 1.06              |
| 5:P:155:PRO:HA       | 14:W:765:LYS:CE     | 1.84                     | 1.06              |
| 5:P:318:THR:HG22     | 13:V:763:LYS:HZ1    | 0.95                     | 1.06              |
| 5:P:324:ALA:HB3      | 13:V:771:GLN:OE1    | 1.55                     | 1.06              |
| 7:Q:124:PHE:CE1      | 7:Q:125:TYR:CZ      | 2.41                     | 1.06              |
| 9:K:1232:LEU:CD2     | 9:K:1265:ILE:CG2    | 2.29                     | 1.06              |
| 10:C16:386:ASN:O     | 10:C16:390:HIS:ND1  | 1.89                     | 1.06              |
| 11:A24:156:MET:HA    | 11:A24:555:HIS:CD2  | 1.91                     | 1.06              |
| 11:A24:707:LEU:HG    | 11:A24:767:ARG:HH22 | 1.12                     | 1.06              |
| 11:A24:806:GLN:OE1   | 11:A24:847:ARG:NH2  | 1.87                     | 1.06              |
| 12:A:206:VAL:HG12    | 12:A:233:ALA:HB1    | 1.35                     | 1.06              |
| 12:A:362:ARG:CD      | 12:A:366:ARG:NH2    | 2.18                     | 1.06              |
| 10:C:1251:PHE:CE2    | 10:C:1319:ARG:NH1   | 2.24                     | 1.06              |
| 10:C8:62:ILE:HD12    | 10:C8:72:LEU:HD11   | 1.31                     | 1.06              |
| 18:B8:262:HIS:ND1    | 18:B8:379:LEU:HD21  | 1.69                     | 1.06              |
| 20:E:353:ILE:HD11    | 20:E:413:PHE:HA     | 1.07                     | 1.06              |
| 19:48:250:ILE:HG23   | 20:E8:165:ARG:NH2   | 1.65                     | 1.06              |
| 22:I16:146:SER:HB3   | 23:J16:574:ARG:NH1  | 1.69                     | 1.06              |
| 22:I16:146:SER:HB3   | 23:J16:574:ARG:HH12 | 0.92                     | 1.06              |
| 24:D:405:GLN:CD      | 24:D16:10:ARG:CZ    | 2.27                     | 1.06              |
| 1:R8:1466:LYS:CG     | 6:O8:160:LEU:HD22   | 1.84                     | 1.06              |
| 2:M8:363:ARG:NH1     | 2:M8:494:SER:O      | 1.87                     | 1.06              |
| 2:M8:627:TYR:CD2     | 3:N8:167:LEU:HA     | 1.90                     | 1.06              |
| 2:M16:363:ARG:NH1    | 2:M16:494:SER:O     | 1.87                     | 1.06              |
| 5:P:155:PRO:CA       | 14:W:765:LYS:HE3    | 1.85                     | 1.06              |
| 5:P:600:PHE:CD2      | 5:P:638:SER:HB2     | 1.76                     | 1.06              |
| 9:K:1180:TRP:CD1     | 9:K:1261:MET:HE2    | 1.89                     | 1.06              |
| 9:K8:716:ALA:HB1     | 10:C32:503:THR:HB   | 1.09                     | 1.06              |
| 10:C16:667:ILE:HD13  | 10:C16:670:GLU:O    | 1.54                     | 1.06              |
| 10:C16:1126:ASP:OD2  | 24:D8:1069:GLY:HA3  | 1.53                     | 1.06              |
| 10:C24:453:LEU:HD23  | 10:C24:459:LEU:CD1  | 1.86                     | 1.06              |
| 10:C24:1285:VAL:HG23 | 10:C24:1738:MET:CE  | 1.83                     | 1.06              |
| 11:A40:206:VAL:HG12  | 11:A40:233:ALA:HB1  | 1.35                     | 1.06              |
| 11:A40:362:ARG:CD    | 11:A40:366:ARG:NH2  | 2.18                     | 1.06              |
| 12:A:555:HIS:O       | 12:A:557:LEU:N      | 1.87                     | 1.06              |
| 18:B:783:LYS:CE      | 24:D16:1064:GLY:HA2 | 1.85                     | 1.06              |
| 18:B:1256:THR:HG23   | 24:D16:1238:GLU:HG3 | 1.31                     | 1.06              |
| 18:B8:66:ASN:OD1     | 18:B8:84:LYS:NZ     | 1.87                     | 1.06              |
| 19:48:187:SER:O      | 19:48:189:LEU:N     | 1.87                     | 1.06              |
| 20:E8:353:ILE:HD11   | 20:E8:413:PHE:HA    | 1.07                     | 1.06              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 21:H8:255:LEU:CD1    | 23:J8:655:GLU:OE2    | 2.02                     | 1.06              |
| 21:H8:291:VAL:HG12   | 23:J8:657:GLU:HG2    | 1.17                     | 1.06              |
| 10:C32:1251:PHE:CE2  | 10:C32:1319:ARG:NH1  | 2.24                     | 1.06              |
| 1:R:1269:LEU:CD1     | 5:P:684:ARG:HD3      | 1.84                     | 1.06              |
| 5:P:401:ARG:CD       | 5:P:414:VAL:HG11     | 1.85                     | 1.06              |
| 8:L16:1026:ARG:HD2   | 9:K16:1284:MET:CG    | 1.85                     | 1.06              |
| 10:C16:1547:LYS:CD   | 24:D8:1406:SER:H     | 1.67                     | 1.06              |
| 10:C24:768:ARG:CZ    | 10:C24:775:LYS:HG2   | 1.82                     | 1.06              |
| 10:C24:1453:ARG:HH22 | 24:D24:1150:GLY:HA2  | 1.20                     | 1.06              |
| 11:A40:691:ALA:CB    | 24:D24:1397:THR:HG21 | 1.86                     | 1.06              |
| 11:A32:555:HIS:O     | 11:A32:557:LEU:N     | 1.87                     | 1.06              |
| 18:B8:536:ILE:HG23   | 18:B8:545:VAL:HG11   | 1.32                     | 1.06              |
| 18:B8:1119:LYS:O     | 18:B8:1120:THR:C     | 1.93                     | 1.06              |
| 18:B8:1940:ALA:CB    | 18:B8:1950:ILE:HD11  | 1.85                     | 1.06              |
| 20:E8:235:HIS:NE2    | 20:E8:239:LYS:HE3    | 1.70                     | 1.06              |
| 23:J32:718:GLN:CD    | 23:J32:737:TRP:CZ3   | 2.33                     | 1.06              |
| 22:I8:146:SER:HB3    | 23:J8:574:ARG:NH1    | 1.69                     | 1.06              |
| 10:C32:62:ILE:HD12   | 10:C32:72:LEU:HD11   | 1.31                     | 1.06              |
| 1:R:1185:THR:HG21    | 24:D:1462:PHE:HZ     | 0.91                     | 1.05              |
| 2:M8:628:LEU:HD13    | 3:N8:223:GLY:C       | 1.80                     | 1.05              |
| 2:M16:844:VAL:HG21   | 4:T16:660:LEU:HD21   | 1.08                     | 1.05              |
| 5:P16:179:TYR:HE1    | 5:P16:437:GLY:N      | 1.51                     | 1.05              |
| 9:K8:958:MET:HE3     | 9:K8:974:LEU:HD22    | 1.07                     | 1.05              |
| 9:K8:1154:TRP:CH2    | 9:K8:1219:VAL:CG1    | 2.38                     | 1.05              |
| 10:C16:1074:LEU:HD12 | 10:C16:1075:ASP:N    | 1.71                     | 1.05              |
| 10:C16:1548:ILE:CG1  | 24:D8:1407:PHE:CE2   | 2.34                     | 1.05              |
| 11:A24:206:VAL:HG12  | 11:A24:233:ALA:HB1   | 1.35                     | 1.05              |
| 11:A24:468:VAL:CG2   | 24:D16:1103:LEU:CD1  | 2.10                     | 1.05              |
| 10:C24:1050:HIS:CD2  | 10:C24:1086:LYS:HZ2  | 1.70                     | 1.05              |
| 11:A16:362:ARG:CD    | 11:A16:366:ARG:NH2   | 2.18                     | 1.05              |
| 11:A16:519:MET:HE1   | 11:A16:569:MET:HE3   | 1.15                     | 1.05              |
| 18:B:686:LEU:CD1     | 18:B:790:ASP:OD2     | 2.03                     | 1.05              |
| 18:B:1119:LYS:O      | 18:B:1120:THR:C      | 1.93                     | 1.05              |
| 18:B8:235:ARG:NH1    | 18:B8:308:GLU:OE2    | 1.89                     | 1.05              |
| 18:B8:771:MET:HE3    | 18:B8:840:VAL:HG11   | 1.38                     | 1.05              |
| 2:M8:844:VAL:HG22    | 4:T8:660:LEU:HD21    | 1.07                     | 1.05              |
| 5:P:109:ILE:CD1      | 14:W:18:PRO:HG3      | 1.82                     | 1.05              |
| 5:P:214:LEU:HD23     | 5:P:236:VAL:CG1      | 1.85                     | 1.05              |
| 5:P8:267:ARG:HH21    | 5:P8:270:GLU:CD      | 1.64                     | 1.05              |
| 8:L16:976:LEU:HD22   | 9:K16:1004:ARG:HD3   | 1.33                     | 1.05              |
| 9:K:635:ALA:HA       | 9:K:655:GLN:HE22     | 1.16                     | 1.05              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K:840:TRP:CZ3     | 9:K:907:ILE:CD1      | 2.34                     | 1.05              |
| 9:K8:1074:ARG:HD2   | 9:K8:1126:LEU:HD21   | 1.33                     | 1.05              |
| 10:C16:1814:LYS:HZ1 | 23:J32:738:MET:HB3   | 0.94                     | 1.05              |
| 11:A40:798:PHE:CZ   | 11:A40:847:ARG:NH1   | 2.25                     | 1.05              |
| 12:A:798:PHE:CZ     | 12:A:847:ARG:NH1     | 2.25                     | 1.05              |
| 10:C:18:THR:HG23    | 10:C:883:GLU:HG2     | 1.36                     | 1.05              |
| 10:C:281:ASP:OD2    | 24:D:1398:ARG:HD2    | 1.53                     | 1.05              |
| 11:A32:90:PHE:CD2   | 18:B8:1788:ILE:CG2   | 2.33                     | 1.05              |
| 11:A32:798:PHE:CZ   | 11:A32:847:ARG:NH1   | 2.25                     | 1.05              |
| 18:B:712:PRO:CG     | 18:B:759:MET:HE2     | 1.78                     | 1.05              |
| 18:B:1439:LYS:HD3   | 24:D16:1257:ASN:HD21 | 1.16                     | 1.05              |
| 18:B8:421:ASP:OD1   | 18:B8:468:ARG:CZ     | 2.03                     | 1.05              |
| 19:4:250:ILE:HG23   | 20:E:165:ARG:NH2     | 1.65                     | 1.05              |
| 23:J8:718:GLN:CD    | 23:J8:737:TRP:CZ3    | 2.33                     | 1.05              |
| 24:D:405:GLN:CB     | 24:D16:10:ARG:HH11   | 1.67                     | 1.05              |
| 12:A48:362:ARG:CD   | 12:A48:366:ARG:NH2   | 2.18                     | 1.05              |
| 12:A48:555:HIS:O    | 12:A48:557:LEU:N     | 1.87                     | 1.05              |
| 1:R16:1101:ARG:NH1  | 1:R16:1188:TYR:CE2   | 2.24                     | 1.05              |
| 5:P:313:TRP:HZ2     | 5:P:345:MET:HE3      | 1.22                     | 1.05              |
| 5:P8:592:SER:OG     | 5:P8:598:LEU:CD1     | 2.05                     | 1.05              |
| 11:A40:468:VAL:HG22 | 24:D32:1103:LEU:HD11 | 1.33                     | 1.05              |
| 10:C:667:ILE:HD13   | 10:C:670:GLU:O       | 1.54                     | 1.05              |
| 10:C:768:ARG:CZ     | 10:C:775:LYS:HG2     | 1.82                     | 1.05              |
| 10:C8:1290:HIS:CG   | 10:C8:1334:MET:HE3   | 1.91                     | 1.05              |
| 11:A16:798:PHE:CZ   | 11:A16:847:ARG:NH1   | 2.25                     | 1.05              |
| 11:A32:206:VAL:HG12 | 11:A32:233:ALA:HB1   | 1.35                     | 1.05              |
| 18:B:783:LYS:HE3    | 24:D16:1064:GLY:HA2  | 1.11                     | 1.05              |
| 18:B8:686:LEU:CD1   | 18:B8:790:ASP:OD2    | 2.03                     | 1.05              |
| 22:I:146:SER:HB3    | 23:J32:574:ARG:HH12  | 0.92                     | 1.05              |
| 22:I:199:PHE:HB2    | 23:J32:620:MET:SD    | 1.97                     | 1.05              |
| 22:I16:199:PHE:HB2  | 23:J16:620:MET:SD    | 1.97                     | 1.05              |
| 10:C32:407:LYS:CG   | 10:C32:465:PHE:CZ    | 2.38                     | 1.05              |
| 12:A48:798:PHE:CZ   | 12:A48:847:ARG:NH1   | 2.25                     | 1.05              |
| 5:P16:592:SER:OG    | 5:P16:598:LEU:CD1    | 2.05                     | 1.05              |
| 9:K:958:MET:HE3     | 9:K:974:LEU:HD22     | 1.07                     | 1.05              |
| 9:K16:894:LYS:NZ    | 9:K16:1057:GLU:CB    | 2.19                     | 1.05              |
| 10:C16:1251:PHE:CE2 | 10:C16:1319:ARG:NH1  | 2.24                     | 1.05              |
| 11:A24:798:PHE:CZ   | 11:A24:847:ARG:NH1   | 2.25                     | 1.05              |
| 10:C24:667:ILE:HD12 | 10:C24:697:HIS:CE1   | 1.90                     | 1.05              |
| 10:C24:847:ARG:HD2  | 10:C24:911:ILE:HD13  | 1.38                     | 1.05              |
| 14:W:598:ILE:HG23   | 14:W:626:LEU:HD22    | 1.30                     | 1.05              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:453:LEU:HD23   | 10:C:459:LEU:CD1     | 1.86                     | 1.05              |
| 11:A16:676:TYR:CZ   | 24:D16:1395:SER:CB   | 2.39                     | 1.05              |
| 11:A32:703:ALA:HA   | 24:D32:1398:ARG:HD3  | 1.31                     | 1.05              |
| 18:B:421:ASP:OD1    | 18:B:468:ARG:CZ      | 2.03                     | 1.05              |
| 18:B:1110:LEU:CD2   | 21:H:326:GLY:N       | 2.20                     | 1.05              |
| 22:I8:199:PHE:HB2   | 23:J8:620:MET:SD     | 1.97                     | 1.05              |
| 21:H24:285:THR:HA   | 23:J24:650:GLN:NE2   | 1.71                     | 1.05              |
| 2:M:428:SER:HB2     | 8:L:355:SER:OG       | 1.56                     | 1.05              |
| 5:P8:15:LEU:HD22    | 6:O8:309:SER:O       | 1.53                     | 1.05              |
| 8:L:1077:LEU:HD13   | 9:K:1086:VAL:HG12    | 1.32                     | 1.05              |
| 8:L16:1096:GLU:OE1  | 9:K16:998:GLN:NE2    | 1.89                     | 1.05              |
| 9:K:635:ALA:HA      | 9:K:655:GLN:NE2      | 1.71                     | 1.05              |
| 9:K:1153:ALA:O      | 9:K:1220:ASN:ND2     | 1.88                     | 1.05              |
| 9:K8:919:MET:SD     | 9:K8:923:ILE:CD1     | 2.45                     | 1.05              |
| 9:K8:1153:ALA:O     | 9:K8:1220:ASN:ND2    | 1.88                     | 1.05              |
| 10:C24:1688:ARG:HG3 | 23:J24:735:LYS:HE3   | 1.33                     | 1.05              |
| 10:C8:453:LEU:HD23  | 10:C8:459:LEU:CD1    | 1.86                     | 1.05              |
| 10:C8:1251:PHE:CE2  | 10:C8:1319:ARG:NH1   | 2.24                     | 1.05              |
| 11:A32:137:GLU:HG3  | 18:B8:1901:GLN:HE22  | 0.90                     | 1.05              |
| 11:A32:440:LEU:CD1  | 11:A32:443:LEU:HD11  | 1.87                     | 1.05              |
| 18:B:1164:GLU:OE1   | 18:B:1399:ILE:HG21   | 1.57                     | 1.05              |
| 18:B8:1161:LEU:CD1  | 18:B8:1403:ILE:HG21  | 1.86                     | 1.05              |
| 18:B8:1256:THR:HG21 | 24:D32:1238:GLU:HG3  | 1.10                     | 1.05              |
| 19:48:250:ILE:HG23  | 20:E8:165:ARG:HH22   | 0.89                     | 1.05              |
| 22:I8:146:SER:HB3   | 23:J8:574:ARG:HH12   | 0.92                     | 1.05              |
| 22:I16:199:PHE:CD1  | 23:J16:620:MET:HG3   | 1.92                     | 1.05              |
| 2:M:628:LEU:HD12    | 3:N:223:GLY:HA3      | 1.38                     | 1.04              |
| 2:M8:851:LEU:HD21   | 4:T8:653:GLN:HG2     | 1.32                     | 1.04              |
| 2:M16:628:LEU:HD13  | 3:N16:223:GLY:C      | 1.80                     | 1.04              |
| 2:M16:628:LEU:HD12  | 3:N16:223:GLY:HA3    | 1.38                     | 1.04              |
| 5:P8:614:VAL:HG23   | 5:P8:629:ARG:NH2     | 1.72                     | 1.04              |
| 8:L16:1030:LEU:HD13 | 9:K16:1285:GLU:HB2   | 1.09                     | 1.04              |
| 10:C16:453:LEU:HD23 | 10:C16:459:LEU:CD1   | 1.86                     | 1.04              |
| 10:C16:667:ILE:HG23 | 10:C16:669:GLY:C     | 1.80                     | 1.04              |
| 10:C16:1664:SER:HA  | 10:C24:1568:ARG:HH21 | 0.93                     | 1.04              |
| 11:A24:519:MET:CE   | 11:A24:569:MET:CE    | 2.31                     | 1.04              |
| 10:C24:1251:PHE:CE2 | 10:C24:1319:ARG:NH1  | 2.24                     | 1.04              |
| 10:C:611:TRP:CH2    | 10:C:670:GLU:OE2     | 2.10                     | 1.04              |
| 10:C:1271:PHE:HZ    | 10:C:1284:ASP:OD1    | 1.40                     | 1.04              |
| 11:A16:676:TYR:HE2  | 24:D16:1396:PRO:CD   | 1.69                     | 1.04              |
| 11:A32:714:GLY:CA   | 24:D32:1398:ARG:NH2  | 2.20                     | 1.04              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:1028:LYS:CE    | 18:B:1092:GLU:OE2   | 2.05                     | 1.04              |
| 18:B8:1164:GLU:OE1  | 18:B8:1399:ILE:HG21 | 1.57                     | 1.04              |
| 20:E8:434:TRP:NE1   | 24:D40:72:GLU:OE2   | 1.89                     | 1.04              |
| 22:I:199:PHE:CD1    | 23:J32:620:MET:HG3  | 1.92                     | 1.04              |
| 22:I8:199:PHE:CD1   | 23:J8:620:MET:HG3   | 1.92                     | 1.04              |
| 24:D:400:VAL:HB     | 24:D16:751:MET:HE2  | 1.32                     | 1.04              |
| 12:A48:206:VAL:HG12 | 12:A48:233:ALA:HB1  | 1.35                     | 1.04              |
| 2:M:342:VAL:HG12    | 2:M:343:MET:H       | 1.20                     | 1.04              |
| 2:M:672:TYR:HB3     | 2:M:680:LYS:HD2     | 1.06                     | 1.04              |
| 1:R8:768:LEU:CG     | 24:D40:1362:VAL:O   | 2.06                     | 1.04              |
| 2:M8:669:ALA:HB2    | 2:M8:684:GLN:CG     | 1.59                     | 1.04              |
| 6:O:82:LEU:HD23     | 6:O:103:MET:HE3     | 1.08                     | 1.04              |
| 5:P16:267:ARG:HH21  | 5:P16:270:GLU:CD    | 1.64                     | 1.04              |
| 9:K8:635:ALA:HA     | 9:K8:655:GLN:NE2    | 1.71                     | 1.04              |
| 10:C16:62:ILE:HD12  | 10:C16:72:LEU:CD1   | 1.87                     | 1.04              |
| 11:A24:160:THR:C    | 11:A24:491:PRO:HG2  | 1.82                     | 1.04              |
| 10:C24:611:TRP:CH2  | 10:C24:670:GLU:OE2  | 2.10                     | 1.04              |
| 10:C24:1688:ARG:CG  | 23:J24:735:LYS:HE3  | 1.86                     | 1.04              |
| 10:C:18:THR:CG2     | 10:C:883:GLU:HG2    | 1.87                     | 1.04              |
| 10:C:453:LEU:HD13   | 10:C:486:LEU:HD21   | 1.39                     | 1.04              |
| 10:C:667:ILE:HG23   | 10:C:669:GLY:C      | 1.80                     | 1.04              |
| 10:C:960:PHE:CZ     | 10:C:1138:GLU:OE2   | 2.09                     | 1.04              |
| 11:A16:206:VAL:HG12 | 11:A16:233:ALA:HB1  | 1.35                     | 1.04              |
| 11:A16:326:TYR:CE1  | 17:F8:77:TYR:CB     | 2.40                     | 1.04              |
| 18:B8:1749:LEU:O    | 18:B8:1781:VAL:HG13 | 1.57                     | 1.04              |
| 19:48:250:ILE:HD11  | 20:E8:163:ILE:HD13  | 1.34                     | 1.04              |
| 20:E8:358:GLY:HA3   | 20:E8:454:MET:SD    | 1.97                     | 1.04              |
| 10:C32:611:TRP:CH2  | 10:C32:670:GLU:OE2  | 2.10                     | 1.04              |
| 12:A48:440:LEU:CD1  | 12:A48:443:LEU:HD11 | 1.87                     | 1.04              |
| 1:R:1166:ASN:ND2    | 5:P:672:LEU:HD22    | 1.71                     | 1.04              |
| 1:R:1269:LEU:CD1    | 5:P:684:ARG:HG2     | 1.85                     | 1.04              |
| 2:M8:628:LEU:HD12   | 3:N8:223:GLY:HA3    | 1.38                     | 1.04              |
| 2:M8:672:TYR:CB     | 2:M8:680:LYS:HD3    | 1.65                     | 1.04              |
| 5:P:267:ARG:HH21    | 5:P:270:GLU:CD      | 1.64                     | 1.04              |
| 7:Q:297:VAL:HG11    | 7:Q:301:ARG:HB2     | 1.33                     | 1.04              |
| 6:O8:82:LEU:HD23    | 6:O8:103:MET:HE3    | 1.08                     | 1.04              |
| 8:L16:605:MET:SD    | 8:L16:631:LEU:HD11  | 1.97                     | 1.04              |
| 9:K8:894:LYS:HD2    | 9:K8:1058:GLU:HG2   | 1.32                     | 1.04              |
| 9:K8:1154:TRP:CZ2   | 9:K8:1219:VAL:CG1   | 2.40                     | 1.04              |
| 10:C16:64:LEU:HD22  | 10:C16:96:ARG:HG3   | 1.38                     | 1.04              |
| 10:C16:557:VAL:HG22 | 10:C16:565:ARG:HH21 | 0.93                     | 1.04              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C16:667:ILE:HD12 | 10:C16:697:HIS:CE1  | 1.90                     | 1.04              |
| 10:C24:64:LEU:HD22  | 10:C24:96:ARG:HG3   | 1.38                     | 1.04              |
| 10:C24:1290:HIS:CG  | 10:C24:1334:MET:HE3 | 1.91                     | 1.04              |
| 10:C24:1548:ILE:CD1 | 24:D24:1407:PHE:HZ  | 1.59                     | 1.04              |
| 12:A:440:LEU:CD1    | 12:A:443:LEU:HD11   | 1.87                     | 1.04              |
| 10:C:565:ARG:HD3    | 10:C:568:TRP:CE3    | 1.85                     | 1.04              |
| 10:C:1290:HIS:CG    | 10:C:1334:MET:HE3   | 1.91                     | 1.04              |
| 10:C8:668:ALA:CA    | 10:C8:700:MET:HE1   | 1.87                     | 1.04              |
| 18:B:1772:HIS:CD2   | 18:B:1878:GLU:OE2   | 2.10                     | 1.04              |
| 18:B8:1291:LEU:CD1  | 18:B8:1332:VAL:HG21 | 1.88                     | 1.04              |
| 19:4:189:LEU:CD1    | 19:4:203:LEU:HD23   | 1.88                     | 1.04              |
| 20:E:353:ILE:CG2    | 20:E:413:PHE:HE2    | 1.70                     | 1.04              |
| 20:E:358:GLY:HA3    | 20:E:454:MET:SD     | 1.97                     | 1.04              |
| 21:H:285:THR:HA     | 23:J32:650:GLN:NE2  | 1.71                     | 1.04              |
| 23:J32:718:GLN:NE2  | 23:J32:737:TRP:HZ3  | 1.32                     | 1.04              |
| 10:C32:62:ILE:HD12  | 10:C32:72:LEU:CD1   | 1.87                     | 1.04              |
| 10:C32:962:PHE:CZ   | 10:C32:997:ILE:HD12 | 1.93                     | 1.04              |
| 2:M:210:GLN:CD      | 10:C:529:GLN:NE2    | 2.16                     | 1.04              |
| 2:M8:844:VAL:HG21   | 4:T8:660:LEU:HD21   | 1.08                     | 1.04              |
| 5:P:57:PRO:CB       | 6:O:29:LEU:CD1      | 2.36                     | 1.04              |
| 5:P16:57:PRO:CB     | 6:O16:29:LEU:CD1    | 2.36                     | 1.04              |
| 5:P16:313:TRP:HZ2   | 5:P16:345:MET:HE3   | 1.22                     | 1.04              |
| 10:C24:62:ILE:HD12  | 10:C24:72:LEU:CD1   | 1.87                     | 1.04              |
| 11:A40:440:LEU:CD1  | 11:A40:443:LEU:HD11 | 1.87                     | 1.04              |
| 13:V:910:GLU:HG3    | 14:W:787:MET:HE1    | 1.37                     | 1.04              |
| 10:C8:62:ILE:HD12   | 10:C8:72:LEU:CD1    | 1.88                     | 1.04              |
| 10:C8:1271:PHE:HZ   | 10:C8:1284:ASP:OD1  | 1.40                     | 1.04              |
| 18:B:1156:GLN:CA    | 18:B:1382:LYS:HZ1   | 1.71                     | 1.04              |
| 21:H:322:LEU:HD13   | 23:J32:689:LEU:CD2  | 1.88                     | 1.04              |
| 21:H8:285:THR:HA    | 23:J8:650:GLN:NE2   | 1.71                     | 1.04              |
| 1:R:1424:LYS:CD     | 6:O:107:SER:OG      | 2.04                     | 1.04              |
| 1:R:1428:VAL:CG2    | 6:O:165:LYS:NZ      | 2.19                     | 1.04              |
| 1:R16:1223:PHE:CD1  | 5:P16:676:GLN:NE2   | 2.26                     | 1.04              |
| 5:P8:313:TRP:HZ2    | 5:P8:345:MET:HE3    | 1.22                     | 1.04              |
| 9:K8:635:ALA:HA     | 9:K8:655:GLN:HE22   | 1.16                     | 1.04              |
| 11:A24:560:MET:HE1  | 11:A24:615:GLN:NE2  | 1.71                     | 1.04              |
| 10:C:407:LYS:HD2    | 10:C:465:PHE:CZ     | 1.88                     | 1.04              |
| 10:C:668:ALA:CA     | 10:C:700:MET:HE1    | 1.88                     | 1.04              |
| 10:C8:453:LEU:HD13  | 10:C8:486:LEU:HD21  | 1.39                     | 1.04              |
| 10:C8:1050:HIS:CD2  | 10:C8:1086:LYS:HZ2  | 1.72                     | 1.04              |
| 18:B:1028:LYS:HE3   | 18:B:1092:GLU:OE2   | 1.58                     | 1.04              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:1161:LEU:CD1    | 18:B:1403:ILE:HG21   | 1.86                     | 1.04              |
| 10:C32:1285:VAL:HG23 | 10:C32:1738:MET:CE   | 1.82                     | 1.04              |
| 1:R:768:LEU:CD1      | 24:D:1362:VAL:O      | 2.05                     | 1.03              |
| 2:M16:816:ARG:HH12   | 2:M16:849:LEU:HB3    | 0.87                     | 1.03              |
| 5:P:467:GLN:NE2      | 6:O:291:SER:HB3      | 1.73                     | 1.03              |
| 5:P:592:SER:OG       | 5:P:598:LEU:CD1      | 2.05                     | 1.03              |
| 10:C16:768:ARG:CZ    | 10:C16:775:LYS:HG2   | 1.82                     | 1.03              |
| 11:A24:440:LEU:CD1   | 11:A24:443:LEU:HD11  | 1.87                     | 1.03              |
| 10:C24:962:PHE:CZ    | 10:C24:997:ILE:HD12  | 1.92                     | 1.03              |
| 11:A40:156:MET:HG2   | 11:A40:555:HIS:CE1   | 1.78                     | 1.03              |
| 19:4:250:ILE:HG23    | 20:E:165:ARG:HH22    | 0.89                     | 1.03              |
| 20:E:49:THR:HG23     | 20:E:121:VAL:HG12    | 1.36                     | 1.03              |
| 22:I24:199:PHE:CD1   | 23:J24:620:MET:HG3   | 1.92                     | 1.03              |
| 10:C32:637:TYR:OH    | 10:C32:642:GLU:OE2   | 1.77                     | 1.03              |
| 10:C32:679:ARG:HH22  | 10:C32:690:LEU:HD21  | 0.93                     | 1.03              |
| 10:C32:1290:HIS:CG   | 10:C32:1334:MET:HE3  | 1.91                     | 1.03              |
| 1:R:1022:TYR:OH      | 24:D:1441:PRO:CB     | 2.06                     | 1.03              |
| 1:R:1033:LYS:HE3     | 24:D:1436:ARG:NH2    | 1.72                     | 1.03              |
| 1:R:1191:LYS:HB2     | 24:D:1453:GLU:HG2    | 1.37                     | 1.03              |
| 3:N16:162:THR:HG23   | 3:N16:168:VAL:HG22   | 1.28                     | 1.03              |
| 5:P16:15:LEU:HD22    | 6:O16:309:SER:O      | 1.53                     | 1.03              |
| 8:L16:1096:GLU:CD    | 9:K16:998:GLN:HG2    | 1.82                     | 1.03              |
| 10:C16:1290:HIS:CG   | 10:C16:1334:MET:HE3  | 1.91                     | 1.03              |
| 10:C16:1688:ARG:CG   | 23:J32:735:LYS:HE3   | 1.87                     | 1.03              |
| 10:C:565:ARG:HD2     | 10:C:568:TRP:CE3     | 1.86                     | 1.03              |
| 10:C8:664:ASN:HA     | 10:C8:667:ILE:HG12   | 1.37                     | 1.03              |
| 11:A16:90:PHE:CD2    | 18:B:1788:ILE:HG21   | 1.84                     | 1.03              |
| 11:A16:440:LEU:CD1   | 11:A16:443:LEU:HD11  | 1.87                     | 1.03              |
| 11:A16:676:TYR:CE2   | 24:D16:1396:PRO:CD   | 2.40                     | 1.03              |
| 11:A16:714:GLY:HA3   | 24:D16:1398:ARG:NH2  | 1.73                     | 1.03              |
| 11:A32:714:GLY:HA3   | 24:D32:1398:ARG:NH2  | 1.74                     | 1.03              |
| 18:B:583:ARG:CZ      | 18:B:711:CYS:HB2     | 1.87                     | 1.03              |
| 18:B:1110:LEU:HD12   | 21:H:323:TYR:OH      | 1.55                     | 1.03              |
| 18:B8:671:MET:CE     | 18:B8:736:ALA:CB     | 2.36                     | 1.03              |
| 18:B8:729:LEU:HB2    | 18:B8:1196:MET:CE    | 1.88                     | 1.03              |
| 18:B8:1028:LYS:CE    | 18:B8:1092:GLU:OE2   | 2.05                     | 1.03              |
| 18:B8:1772:HIS:CD2   | 18:B8:1878:GLU:OE2   | 2.10                     | 1.03              |
| 10:C32:847:ARG:HD2   | 10:C32:911:ILE:CD1   | 1.89                     | 1.03              |
| 10:C32:1348:LEU:HD12 | 10:C32:1359:ILE:HD11 | 1.03                     | 1.03              |
| 2:M:399:THR:OG1      | 2:M:480:ARG:NH2      | 1.92                     | 1.03              |
| 1:R8:1449:TRP:CH2    | 2:M8:161:ASP:O       | 2.12                     | 1.03              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:N8:162:THR:CG2    | 3:N8:168:VAL:HG22   | 1.83                     | 1.03              |
| 2:M16:351:ALA:HB1   | 8:L16:219:ILE:HG21  | 1.10                     | 1.03              |
| 10:C16:637:TYR:OH   | 10:C16:642:GLU:OE2  | 1.77                     | 1.03              |
| 10:C16:962:PHE:CZ   | 10:C16:997:ILE:HD12 | 1.93                     | 1.03              |
| 11:A24:468:VAL:HG21 | 24:D16:1100:GLN:CD  | 1.83                     | 1.03              |
| 10:C24:390:HIS:CG   | 10:C24:452:LEU:HB2  | 1.93                     | 1.03              |
| 11:A40:326:TYR:CE1  | 17:F16:77:TYR:CB    | 2.40                     | 1.03              |
| 18:B:1749:LEU:O     | 18:B:1781:VAL:HG13  | 1.58                     | 1.03              |
| 18:B8:864:LEU:O     | 18:B8:910:TYR:OH    | 1.74                     | 1.03              |
| 20:E8:123:CYS:SG    | 20:E8:135:ILE:HD12  | 1.95                     | 1.03              |
| 20:E8:353:ILE:CG2   | 20:E8:413:PHE:HE2   | 1.70                     | 1.03              |
| 21:H24:322:LEU:HD13 | 23:J24:689:LEU:CD2  | 1.88                     | 1.03              |
| 1:R:1187:ARG:NH2    | 1:R:1201:LEU:HD11   | 1.74                     | 1.03              |
| 2:M:627:TYR:CE2     | 3:N:166:ALA:N       | 2.26                     | 1.03              |
| 1:R8:1165:MET:SD    | 5:P8:676:GLN:NE2    | 2.32                     | 1.03              |
| 2:M8:385:LEU:HD11   | 2:M8:396:PHE:CE2    | 1.94                     | 1.03              |
| 2:M8:534:HIS:CD2    | 2:M8:557:THR:HG22   | 1.94                     | 1.03              |
| 2:M16:417:ARG:NH2   | 8:L16:411:GLU:OE1   | 1.89                     | 1.03              |
| 7:Q:241:HIS:NE2     | 7:Q:258:ARG:NH2     | 2.07                     | 1.03              |
| 10:C16:620:PRO:CB   | 10:C16:636:VAL:CG1  | 2.36                     | 1.03              |
| 10:C24:1453:ARG:CZ  | 24:D24:1150:GLY:HA3 | 1.86                     | 1.03              |
| 10:C:847:ARG:HD2    | 10:C:911:ILE:HD13   | 1.38                     | 1.03              |
| 10:C8:637:TYR:OH    | 10:C8:642:GLU:OE2   | 1.77                     | 1.03              |
| 18:B:671:MET:CE     | 18:B:736:ALA:CB     | 2.36                     | 1.03              |
| 18:B:1291:LEU:CD1   | 18:B:1332:VAL:HG21  | 1.88                     | 1.03              |
| 19:48:189:LEU:CD1   | 19:48:203:LEU:HD23  | 1.88                     | 1.03              |
| 21:H16:285:THR:HA   | 23:J16:650:GLN:NE2  | 1.71                     | 1.03              |
| 21:H16:285:THR:HA   | 23:J16:650:GLN:HE22 | 0.87                     | 1.03              |
| 24:D:387:LEU:HB2    | 24:D16:746:ALA:HB2  | 1.39                     | 1.03              |
| 10:C32:390:HIS:ND1  | 10:C32:452:LEU:HB3  | 1.73                     | 1.03              |
| 10:C32:620:PRO:CB   | 10:C32:636:VAL:CG1  | 2.36                     | 1.03              |
| 2:M:385:LEU:HD11    | 2:M:396:PHE:CE2     | 1.94                     | 1.03              |
| 1:R8:1466:LYS:HD2   | 6:O8:160:LEU:HB2    | 1.40                     | 1.03              |
| 2:M16:399:THR:OG1   | 2:M16:480:ARG:NH2   | 1.92                     | 1.03              |
| 2:M16:416:VAL:HG11  | 8:L16:398:ALA:HB2   | 1.35                     | 1.03              |
| 5:P8:57:PRO:CB      | 6:O8:29:LEU:CD1     | 2.36                     | 1.03              |
| 6:O8:179:LYS:HD3    | 6:O8:183:GLN:OE1    | 0.85                     | 1.03              |
| 7:Q8:241:HIS:NE2    | 7:Q8:258:ARG:NH2    | 2.07                     | 1.03              |
| 6:O16:179:LYS:HD3   | 6:O16:183:GLN:OE1   | 0.85                     | 1.03              |
| 8:L16:1030:LEU:HD22 | 9:K16:1285:GLU:CD   | 1.83                     | 1.03              |
| 9:K8:716:ALA:HB1    | 10:C32:503:THR:CB   | 1.87                     | 1.03              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:611:TRP:CH2   | 10:C16:670:GLU:OE2   | 2.10                     | 1.03              |
| 10:C16:847:ARG:HD2   | 10:C16:911:ILE:CD1   | 1.89                     | 1.03              |
| 11:A24:607:ARG:NH2   | 24:D16:914:PHE:CD1   | 2.26                     | 1.03              |
| 10:C24:1271:PHE:HZ   | 10:C24:1284:ASP:OD1  | 1.40                     | 1.03              |
| 10:C24:1814:LYS:HE2  | 23:J24:738:MET:CE    | 1.89                     | 1.03              |
| 13:V:815:TYR:OH      | 15:J:627:ILE:CD1     | 2.06                     | 1.03              |
| 14:W:781:LEU:HD21    | 15:J:695:ILE:HG21    | 1.38                     | 1.03              |
| 10:C:1348:LEU:HD12   | 10:C:1359:ILE:HD11   | 1.03                     | 1.03              |
| 10:C8:611:TRP:CH2    | 10:C8:670:GLU:OE2    | 2.10                     | 1.03              |
| 11:A32:90:PHE:CZ     | 18:B8:1788:ILE:HG23  | 1.92                     | 1.03              |
| 11:A32:326:TYR:CE1   | 17:F24:77:TYR:CB     | 2.40                     | 1.03              |
| 11:A32:362:ARG:CD    | 11:A32:366:ARG:HH22  | 1.72                     | 1.03              |
| 18:B:729:LEU:HB2     | 18:B:1196:MET:CE     | 1.88                     | 1.03              |
| 21:H24:285:THR:HA    | 23:J24:650:GLN:HE22  | 0.87                     | 1.03              |
| 2:M:816:ARG:HH12     | 2:M:849:LEU:HB3      | 0.87                     | 1.02              |
| 1:R8:1187:ARG:NH2    | 1:R8:1201:LEU:HD11   | 1.74                     | 1.02              |
| 6:O:133:LEU:HD11     | 6:O:153:PHE:CZ       | 1.95                     | 1.02              |
| 5:P8:611:LEU:HG      | 5:P8:629:ARG:HD3     | 1.36                     | 1.02              |
| 6:O8:133:LEU:HD11    | 6:O8:153:PHE:CZ      | 1.95                     | 1.02              |
| 9:K:1154:TRP:CZ2     | 9:K:1219:VAL:CG1     | 2.40                     | 1.02              |
| 10:C16:668:ALA:CA    | 10:C16:700:MET:HE1   | 1.88                     | 1.02              |
| 11:A24:468:VAL:HG22  | 24:D16:1103:LEU:HD11 | 1.38                     | 1.02              |
| 11:A24:737:GLU:CG    | 24:D16:871:ARG:HH21  | 1.71                     | 1.02              |
| 13:V:835:GLU:CG      | 15:J:648:TYR:OH      | 2.07                     | 1.02              |
| 10:C:637:TYR:OH      | 10:C:642:GLU:OE2     | 1.77                     | 1.02              |
| 18:B:514:THR:HG22    | 18:B:549:TRP:CH2     | 1.93                     | 1.02              |
| 18:B:771:MET:HE3     | 18:B:840:VAL:HG11    | 1.39                     | 1.02              |
| 18:B8:583:ARG:CZ     | 18:B8:711:CYS:HB2    | 1.87                     | 1.02              |
| 20:E:123:CYS:SG      | 20:E:135:ILE:HD12    | 1.95                     | 1.02              |
| 20:E8:49:THR:HG23    | 20:E8:121:VAL:HG12   | 1.36                     | 1.02              |
| 21:H8:322:LEU:HD13   | 23:J8:689:LEU:CD2    | 1.88                     | 1.02              |
| 24:D:1009:CYS:O      | 24:D:1013:HIS:ND1    | 1.92                     | 1.02              |
| 24:D8:853:MET:HB3    | 24:D8:885:TYR:CE2    | 1.93                     | 1.02              |
| 24:D40:1109:LEU:HD13 | 24:D40:1127:ARG:HG3  | 1.05                     | 1.02              |
| 10:C32:668:ALA:CA    | 10:C32:700:MET:HE1   | 1.88                     | 1.02              |
| 10:C32:768:ARG:CZ    | 10:C32:775:LYS:HG2   | 1.82                     | 1.02              |
| 12:A48:362:ARG:CD    | 12:A48:366:ARG:HH22  | 1.72                     | 1.02              |
| 1:R:1075:LYS:HE2     | 5:P:713:LEU:C        | 1.85                     | 1.02              |
| 3:N8:4:GLN:NE2       | 3:N8:44:GLY:CA       | 2.23                     | 1.02              |
| 2:M16:639:GLN:HE22   | 3:N16:269:LEU:CD1    | 1.72                     | 1.02              |
| 5:P:16:PHE:CD1       | 6:O:311:LEU:HD11     | 1.94                     | 1.02              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:P:633:LEU:CD2     | 5:P:647:LEU:HD13    | 1.89                     | 1.02              |
| 5:P8:105:ARG:CZ     | 5:P8:130:VAL:HG22   | 1.89                     | 1.02              |
| 5:P8:467:GLN:NE2    | 6:O8:291:SER:HB3    | 1.73                     | 1.02              |
| 6:O16:82:LEU:HD23   | 6:O16:103:MET:HE3   | 1.08                     | 1.02              |
| 9:K8:975:MET:CE     | 9:K8:989:VAL:HG11   | 1.89                     | 1.02              |
| 11:A24:326:TYR:CE1  | 17:F:77:TYR:CB      | 2.40                     | 1.02              |
| 10:C24:407:LYS:CG   | 10:C24:465:PHE:CZ   | 2.38                     | 1.02              |
| 10:C24:1290:HIS:CB  | 10:C24:1334:MET:HE3 | 1.89                     | 1.02              |
| 14:W:515:CYS:HB3    | 14:W:604:PRO:N      | 1.65                     | 1.02              |
| 14:W:584:CYS:SG     | 15:J:573:LYS:CD     | 2.46                     | 1.02              |
| 10:C8:1290:HIS:CB   | 10:C8:1334:MET:HE3  | 1.89                     | 1.02              |
| 18:B8:132:LEU:CD1   | 18:B8:199:LEU:HD11  | 1.89                     | 1.02              |
| 18:B8:712:PRO:CB    | 18:B8:759:MET:HE2   | 1.89                     | 1.02              |
| 22:I:321:LYS:NZ     | 23:J32:711:GLU:OE2  | 1.92                     | 1.02              |
| 22:I24:199:PHE:HB2  | 23:J24:620:MET:SD   | 1.97                     | 1.02              |
| 23:J24:718:GLN:NE2  | 23:J24:737:TRP:HZ3  | 1.31                     | 1.02              |
| 10:C32:64:LEU:HD22  | 10:C32:96:ARG:HG3   | 1.38                     | 1.02              |
| 2:M8:639:GLN:HE22   | 3:N8:269:LEU:CD1    | 1.72                     | 1.02              |
| 2:M8:669:ALA:CB     | 2:M8:684:GLN:CD     | 2.20                     | 1.02              |
| 2:M16:231:ARG:CD    | 2:M16:299:GLY:HA2   | 1.76                     | 1.02              |
| 2:M16:342:VAL:HG12  | 2:M16:343:MET:H     | 1.20                     | 1.02              |
| 5:P:401:ARG:NH2     | 5:P:404:ILE:CG2     | 2.23                     | 1.02              |
| 5:P16:467:GLN:NE2   | 6:O16:291:SER:HB3   | 1.73                     | 1.02              |
| 10:C16:1290:HIS:CB  | 10:C16:1334:MET:HE3 | 1.89                     | 1.02              |
| 10:C24:620:PRO:CB   | 10:C24:636:VAL:CG1  | 2.36                     | 1.02              |
| 10:C24:637:TYR:OH   | 10:C24:642:GLU:OE2  | 1.77                     | 1.02              |
| 10:C24:668:ALA:CA   | 10:C24:700:MET:HE1  | 1.88                     | 1.02              |
| 10:C24:847:ARG:HD2  | 10:C24:911:ILE:CD1  | 1.89                     | 1.02              |
| 14:W:698:LEU:HD12   | 15:J:617:LEU:HD23   | 1.40                     | 1.02              |
| 10:C:620:PRO:CB     | 10:C:636:VAL:CG1    | 2.36                     | 1.02              |
| 10:C8:1348:LEU:HD12 | 10:C8:1359:ILE:HD11 | 1.03                     | 1.02              |
| 11:A16:198:PRO:HB2  | 11:A16:200:HIS:CE1  | 1.95                     | 1.02              |
| 11:A16:703:ALA:HA   | 24:D16:1398:ARG:HD3 | 1.35                     | 1.02              |
| 11:A32:122:LYS:HE3  | 18:B8:1757:GLU:OE1  | 1.56                     | 1.02              |
| 18:B:712:PRO:CB     | 18:B:759:MET:HE2    | 1.89                     | 1.02              |
| 18:B8:1342:LEU:HD23 | 18:B8:1406:ALA:CB   | 1.90                     | 1.02              |
| 20:E:355:PRO:CA     | 20:E:454:MET:HE1    | 1.90                     | 1.02              |
| 20:E:429:PRO:CD     | 24:D:72:GLU:OE2     | 2.08                     | 1.02              |
| 20:E8:353:ILE:HD11  | 20:E8:413:PHE:CA    | 1.89                     | 1.02              |
| 21:H16:322:LEU:HD13 | 23:J16:689:LEU:CD2  | 1.88                     | 1.02              |
| 10:C32:1271:PHE:HZ  | 10:C32:1284:ASP:OD1 | 1.40                     | 1.02              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R:1449:TRP:CH2     | 2:M:161:ASP:O        | 2.12                     | 1.02              |
| 2:M:639:GLN:HE22     | 3:N:269:LEU:CD1      | 1.72                     | 1.02              |
| 2:M16:231:ARG:HD2    | 2:M16:299:GLY:HA3    | 1.04                     | 1.02              |
| 5:P8:16:PHE:CD1      | 6:O8:311:LEU:HD11    | 1.94                     | 1.02              |
| 8:L16:1069:LEU:CD1   | 9:K16:1086:VAL:HG11  | 1.90                     | 1.02              |
| 9:K8:894:LYS:HE2     | 9:K8:1058:GLU:O      | 1.59                     | 1.02              |
| 10:C16:620:PRO:CB    | 10:C16:636:VAL:HG13  | 1.90                     | 1.02              |
| 10:C16:1453:ARG:HH22 | 24:D8:1150:GLY:HA3   | 0.88                     | 1.02              |
| 10:C24:620:PRO:CB    | 10:C24:636:VAL:HG13  | 1.90                     | 1.02              |
| 11:A40:737:GLU:HG3   | 24:D32:871:ARG:HH21  | 1.23                     | 1.02              |
| 14:W:590:LEU:HD11    | 14:W:641:GLU:CD      | 1.83                     | 1.02              |
| 10:C:62:ILE:HD12     | 10:C:72:LEU:CD1      | 1.87                     | 1.02              |
| 10:C8:620:PRO:CB     | 10:C8:636:VAL:CG1    | 2.36                     | 1.02              |
| 18:B:864:LEU:O       | 18:B:910:TYR:OH      | 1.74                     | 1.02              |
| 18:B:1529:GLU:CD     | 24:D16:1415:LEU:CD1  | 2.32                     | 1.02              |
| 18:B8:928:ARG:HH22   | 18:B8:970:SER:HA     | 1.25                     | 1.02              |
| 18:B8:1028:LYS:HE3   | 18:B8:1092:GLU:OE2   | 1.58                     | 1.02              |
| 21:H:285:THR:HA      | 23:J32:650:GLN:HE22  | 0.87                     | 1.02              |
| 10:C32:620:PRO:CB    | 10:C32:636:VAL:HG13  | 1.90                     | 1.02              |
| 2:M:399:THR:CB       | 2:M:480:ARG:NH2      | 2.22                     | 1.02              |
| 2:M8:342:VAL:HG12    | 2:M8:343:MET:H       | 1.20                     | 1.02              |
| 2:M8:399:THR:OG1     | 2:M8:480:ARG:NH2     | 1.92                     | 1.02              |
| 2:M8:816:ARG:HH12    | 2:M8:849:LEU:HB3     | 0.87                     | 1.02              |
| 1:R16:1187:ARG:NH2   | 1:R16:1201:LEU:HD11  | 1.74                     | 1.02              |
| 1:R16:1449:TRP:CH2   | 2:M16:161:ASP:O      | 2.12                     | 1.02              |
| 5:P16:16:PHE:CD1     | 6:O16:311:LEU:HD11   | 1.94                     | 1.02              |
| 9:K:792:LEU:HD11     | 9:K:864:ILE:HD13     | 1.39                     | 1.02              |
| 10:C16:1271:PHE:HZ   | 10:C16:1284:ASP:OD1  | 1.40                     | 1.02              |
| 10:C16:1549:VAL:HG13 | 10:C16:1592:VAL:HG13 | 1.42                     | 1.02              |
| 12:A:198:PRO:HB2     | 12:A:200:HIS:CE1     | 1.95                     | 1.02              |
| 10:C:64:LEU:HD22     | 10:C:96:ARG:HG3      | 1.38                     | 1.02              |
| 10:C8:847:ARG:NH2    | 10:C8:910:SER:HB2    | 1.75                     | 1.02              |
| 11:A16:806:GLN:CD    | 11:A16:847:ARG:NH2   | 2.18                     | 1.02              |
| 18:B8:514:THR:HG22   | 18:B8:549:TRP:CH2    | 1.93                     | 1.02              |
| 18:B8:676:ASP:O      | 18:B8:678:PRO:HD3    | 1.60                     | 1.02              |
| 20:E8:138:ARG:NH2    | 20:E8:190:TYR:CE2    | 2.27                     | 1.02              |
| 21:H8:285:THR:HA     | 23:J8:650:GLN:HE22   | 0.87                     | 1.02              |
| 3:N:158:TRP:CE2      | 3:N:179:LEU:HD21     | 1.95                     | 1.01              |
| 2:M8:672:TYR:HB2     | 2:M8:680:LYS:CD      | 1.68                     | 1.01              |
| 2:M16:385:LEU:HD11   | 2:M16:396:PHE:CE2    | 1.94                     | 1.01              |
| 3:N16:158:TRP:CE2    | 3:N16:179:LEU:HD21   | 1.95                     | 1.01              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:667:ILE:O     | 10:C16:668:ALA:C     | 1.68                     | 1.01              |
| 11:A24:198:PRO:HB2   | 11:A24:200:HIS:CE1   | 1.95                     | 1.01              |
| 10:C24:1348:LEU:HD12 | 10:C24:1359:ILE:HD11 | 1.03                     | 1.01              |
| 10:C:979:MET:CE      | 10:C:1028:ILE:HG21   | 1.88                     | 1.01              |
| 10:C:1290:HIS:CB     | 10:C:1334:MET:HE3    | 1.89                     | 1.01              |
| 10:C8:620:PRO:CB     | 10:C8:636:VAL:HG13   | 1.90                     | 1.01              |
| 10:C8:847:ARG:HD2    | 10:C8:911:ILE:CD1    | 1.89                     | 1.01              |
| 10:C8:1285:VAL:HG23  | 10:C8:1738:MET:CE    | 1.82                     | 1.01              |
| 11:A32:806:GLN:CD    | 11:A32:847:ARG:NH2   | 2.18                     | 1.01              |
| 18:B:729:LEU:HD13    | 18:B:1196:MET:HE1    | 1.42                     | 1.01              |
| 18:B:1342:LEU:HD23   | 18:B:1406:ALA:CB     | 1.90                     | 1.01              |
| 18:B8:1156:GLN:CA    | 18:B8:1382:LYS:HZ1   | 1.73                     | 1.01              |
| 24:D:409:LEU:CD2     | 24:D16:746:ALA:H     | 1.73                     | 1.01              |
| 1:R:983:ARG:NH2      | 24:D:1366:PRO:CD     | 2.23                     | 1.01              |
| 1:R:1033:LYS:NZ      | 24:D:1432:THR:HB     | 1.74                     | 1.01              |
| 2:M:399:THR:CG2      | 2:M:480:ARG:HH21     | 1.72                     | 1.01              |
| 2:M8:544:LEU:HD21    | 2:M8:586:ALA:HB1     | 1.40                     | 1.01              |
| 2:M8:730:GLU:HG3     | 8:L16:504:GLN:NE2    | 1.69                     | 1.01              |
| 6:O:179:LYS:HD3      | 6:O:183:GLN:OE1      | 0.85                     | 1.01              |
| 5:P16:179:TYR:HE1    | 5:P16:436:ALA:C      | 1.56                     | 1.01              |
| 6:O16:133:LEU:HD11   | 6:O16:153:PHE:CZ     | 1.94                     | 1.01              |
| 9:K:1085:TYR:HE1     | 9:K:1093:SER:CA      | 1.69                     | 1.01              |
| 9:K8:1085:TYR:HE1    | 9:K8:1093:SER:CA     | 1.69                     | 1.01              |
| 10:C16:1074:LEU:HD12 | 10:C16:1075:ASP:HA   | 1.02                     | 1.01              |
| 10:C16:1348:LEU:HD12 | 10:C16:1359:ILE:HD11 | 1.03                     | 1.01              |
| 11:A24:362:ARG:CD    | 11:A24:366:ARG:HH22  | 1.72                     | 1.01              |
| 10:C24:1699:LYS:HZ2  | 23:J24:722:LEU:CD2   | 1.65                     | 1.01              |
| 11:A40:198:PRO:HB2   | 11:A40:200:HIS:CE1   | 1.95                     | 1.01              |
| 10:C:667:ILE:HD12    | 10:C:697:HIS:CE1     | 1.91                     | 1.01              |
| 11:A16:90:PHE:CZ     | 18:B:1788:ILE:CG2    | 2.42                     | 1.01              |
| 11:A32:6:GLU:OE1     | 21:H24:332:GLU:OE1   | 1.78                     | 1.01              |
| 18:B:132:LEU:CD1     | 18:B:199:LEU:HD11    | 1.89                     | 1.01              |
| 19:48:342:GLU:OE1    | 24:D8:174:SER:CB     | 2.08                     | 1.01              |
| 22:I16:321:LYS:NZ    | 23:J16:711:GLU:OE2   | 1.92                     | 1.01              |
| 24:D32:642:VAL:HG22  | 24:D40:631:ARG:NH2   | 1.74                     | 1.01              |
| 10:C32:847:ARG:NH2   | 10:C32:910:SER:HB2   | 1.75                     | 1.01              |
| 2:M:254:LEU:HD22     | 2:M:283:ILE:CD1      | 1.90                     | 1.01              |
| 3:N8:158:TRP:CE2     | 3:N8:179:LEU:HD21    | 1.95                     | 1.01              |
| 3:N16:4:GLN:NE2      | 3:N16:44:GLY:CA      | 2.22                     | 1.01              |
| 8:L:1089:MET:HE3     | 9:K:1000:SER:HB2     | 1.37                     | 1.01              |
| 9:K8:649:MET:CB      | 9:K8:704:ARG:NH2     | 2.23                     | 1.01              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:667:ILE:HG23  | 10:C16:670:GLU:N     | 1.76                     | 1.01              |
| 11:A40:468:VAL:CG2   | 24:D32:1103:LEU:CD1  | 2.26                     | 1.01              |
| 11:A16:154:ILE:HD11  | 18:B:1842:VAL:HG13   | 1.41                     | 1.01              |
| 18:B8:917:PHE:HE2    | 18:B8:960:GLN:NE2    | 1.58                     | 1.01              |
| 18:B8:1768:ILE:HG22  | 18:B8:1770:THR:CG2   | 1.89                     | 1.01              |
| 20:E:138:ARG:NH2     | 20:E:190:TYR:CE2     | 2.27                     | 1.01              |
| 21:H:322:LEU:HD13    | 23:J32:689:LEU:HD23  | 1.43                     | 1.01              |
| 22:I8:321:LYS:NZ     | 23:J8:711:GLU:OE2    | 1.92                     | 1.01              |
| 22:I24:321:LYS:NZ    | 23:J24:711:GLU:OE2   | 1.92                     | 1.01              |
| 10:C32:847:ARG:HD2   | 10:C32:911:ILE:HD13  | 1.38                     | 1.01              |
| 12:A48:806:GLN:CD    | 12:A48:847:ARG:NH2   | 2.18                     | 1.01              |
| 1:R:1290:ILE:HD11    | 10:C:605:GLU:CD      | 1.85                     | 1.01              |
| 1:R8:1445:GLU:OE2    | 2:M8:185:ARG:NH2     | 1.94                     | 1.01              |
| 1:R8:1449:TRP:CZ2    | 2:M8:161:ASP:O       | 2.14                     | 1.01              |
| 2:M8:399:THR:CG2     | 2:M8:480:ARG:HH21    | 1.72                     | 1.01              |
| 2:M16:399:THR:CB     | 2:M16:480:ARG:NH2    | 2.22                     | 1.01              |
| 4:T:672:GLN:HG3      | 5:P:702:LEU:CD2      | 1.91                     | 1.01              |
| 7:Q16:241:HIS:NE2    | 7:Q16:258:ARG:NH2    | 2.07                     | 1.01              |
| 8:L16:1096:GLU:OE2   | 9:K16:998:GLN:CG     | 2.08                     | 1.01              |
| 9:K:1198:LEU:CD1     | 9:K:1267:LEU:HD22    | 1.90                     | 1.01              |
| 10:C16:619:LEU:HB3   | 10:C16:620:PRO:HD2   | 1.42                     | 1.01              |
| 10:C16:847:ARG:HD2   | 10:C16:911:ILE:HD13  | 1.38                     | 1.01              |
| 10:C16:1814:LYS:NZ   | 23:J32:738:MET:CB    | 2.21                     | 1.01              |
| 22:I24:131:ARG:HG3   | 23:J24:557:ARG:HH21  | 1.25                     | 1.01              |
| 10:C32:619:LEU:HB3   | 10:C32:620:PRO:HD2   | 1.42                     | 1.01              |
| 3:N:4:GLN:NE2        | 3:N:44:GLY:CA        | 2.23                     | 1.01              |
| 1:R8:1466:LYS:HG2    | 6:O8:160:LEU:HD22    | 1.41                     | 1.01              |
| 2:M8:669:ALA:HB3     | 2:M8:684:GLN:HG3     | 1.39                     | 1.01              |
| 1:R16:1166:ASN:HD21  | 5:P16:672:LEU:HD22   | 1.25                     | 1.01              |
| 5:P8:611:LEU:HG      | 5:P8:629:ARG:CD      | 1.91                     | 1.01              |
| 6:O8:176:ASN:HD21    | 6:O8:179:LYS:HE3     | 1.24                     | 1.01              |
| 5:P16:267:ARG:NH2    | 5:P16:270:GLU:OE1    | 1.94                     | 1.01              |
| 10:C16:453:LEU:HD13  | 10:C16:486:LEU:HD21  | 1.39                     | 1.01              |
| 11:A24:560:MET:HE2   | 11:A24:615:GLN:HE22  | 1.24                     | 1.01              |
| 10:C24:1549:VAL:HG13 | 10:C24:1592:VAL:HG13 | 1.42                     | 1.01              |
| 11:A40:103:GLU:CD    | 21:H16:323:TYR:CE2   | 2.38                     | 1.01              |
| 12:A:362:ARG:CD      | 12:A:366:ARG:HH22    | 1.72                     | 1.01              |
| 13:V:745:LEU:CD1     | 15:J:557:ARG:NH1     | 2.24                     | 1.01              |
| 14:W:659:ARG:HH22    | 15:J:583:LEU:CD2     | 1.73                     | 1.01              |
| 14:W:711:ARG:HD3     | 10:C8:1609:ASP:OD2   | 1.58                     | 1.01              |
| 10:C:620:PRO:CB      | 10:C:636:VAL:HG13    | 1.90                     | 1.01              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:847:ARG:NH2     | 10:C:910:SER:HB2     | 1.75                     | 1.01              |
| 11:A16:362:ARG:CD    | 11:A16:366:ARG:HH22  | 1.72                     | 1.01              |
| 18:B:1110:LEU:CD2    | 21:H:326:GLY:H       | 1.74                     | 1.01              |
| 18:B8:729:LEU:HD13   | 18:B8:1196:MET:HE1   | 1.41                     | 1.01              |
| 19:4:282:GLU:OE1     | 19:4:285:THR:OG1     | 1.78                     | 1.01              |
| 20:E:353:ILE:HD11    | 20:E:413:PHE:CA      | 1.89                     | 1.01              |
| 21:H8:322:LEU:HD13   | 23:J8:689:LEU:HD23   | 1.43                     | 1.01              |
| 10:C32:390:HIS:CG    | 10:C32:452:LEU:HB3   | 1.96                     | 1.01              |
| 10:C32:1549:VAL:HG13 | 10:C32:1592:VAL:HG13 | 1.42                     | 1.01              |
| 12:A48:198:PRO:HB2   | 12:A48:200:HIS:CE1   | 1.95                     | 1.01              |
| 1:R16:1449:TRP:CZ2   | 2:M16:161:ASP:O      | 2.14                     | 1.00              |
| 2:M16:847:PHE:CB     | 4:T16:656:TRP:CE3    | 2.32                     | 1.00              |
| 3:N16:162:THR:CG2    | 3:N16:168:VAL:HG22   | 1.83                     | 1.00              |
| 6:O16:176:ASN:HD21   | 6:O16:179:LYS:HE3    | 1.24                     | 1.00              |
| 11:A40:362:ARG:CD    | 11:A40:366:ARG:HH22  | 1.72                     | 1.00              |
| 11:A40:806:GLN:CD    | 11:A40:847:ARG:NH2   | 2.18                     | 1.00              |
| 12:A:215:ASN:OD1     | 12:A:592:GLN:NE2     | 1.94                     | 1.00              |
| 10:C8:1303:LEU:HD13  | 10:C8:1323:LEU:HD23  | 1.44                     | 1.00              |
| 11:A16:215:ASN:OD1   | 11:A16:592:GLN:NE2   | 1.94                     | 1.00              |
| 20:E8:355:PRO:CA     | 20:E8:454:MET:HE1    | 1.90                     | 1.00              |
| 21:H24:291:VAL:HG12  | 23:J24:657:GLU:CG    | 1.91                     | 1.00              |
| 10:C32:1290:HIS:CB   | 10:C32:1334:MET:HE3  | 1.89                     | 1.00              |
| 9:K:649:MET:CB       | 9:K:704:ARG:NH2      | 2.23                     | 1.00              |
| 9:K:1074:ARG:HD2     | 9:K:1126:LEU:CD2     | 1.91                     | 1.00              |
| 10:C16:1453:ARG:NH2  | 24:D8:1150:GLY:CA    | 2.13                     | 1.00              |
| 11:A24:806:GLN:CD    | 11:A24:847:ARG:NH2   | 2.18                     | 1.00              |
| 12:A:806:GLN:CD      | 12:A:847:ARG:NH2     | 2.18                     | 1.00              |
| 11:A32:198:PRO:HB2   | 11:A32:200:HIS:CE1   | 1.95                     | 1.00              |
| 18:B:917:PHE:HE2     | 18:B:960:GLN:NE2     | 1.58                     | 1.00              |
| 18:B8:94:LEU:HD21    | 18:B8:132:LEU:CD2    | 1.91                     | 1.00              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:HA     | 1.91                     | 1.00              |
| 21:H8:285:THR:CA     | 23:J8:650:GLN:HE22   | 1.74                     | 1.00              |
| 1:R:1445:GLU:OE2     | 2:M:185:ARG:NH2      | 1.94                     | 1.00              |
| 1:R:1449:TRP:HZ3     | 2:M:160:LEU:HD12     | 1.23                     | 1.00              |
| 2:M8:399:THR:CB      | 2:M8:480:ARG:NH2     | 2.22                     | 1.00              |
| 2:M16:399:THR:CG2    | 2:M16:480:ARG:HH21   | 1.72                     | 1.00              |
| 7:Q:327:LEU:HD11     | 7:Q:358:PHE:CE1      | 1.97                     | 1.00              |
| 9:K:1039:ASP:OD1     | 9:K:1096:LYS:NZ      | 1.94                     | 1.00              |
| 9:K8:1198:LEU:CD1    | 9:K8:1267:LEU:HD22   | 1.90                     | 1.00              |
| 10:C16:390:HIS:HB3   | 10:C16:452:LEU:HB2   | 1.43                     | 1.00              |
| 10:C16:407:LYS:CG    | 10:C16:465:PHE:CZ    | 2.38                     | 1.00              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A24:390:ALA:HB1  | 24:D16:1099:ARG:HD3  | 1.38                     | 1.00              |
| 10:C24:667:ILE:HG23 | 10:C24:670:GLU:N     | 1.76                     | 1.00              |
| 12:A:212:LYS:HE2    | 12:A:585:MET:CE      | 1.76                     | 1.00              |
| 11:A16:6:GLU:OE1    | 21:H:332:GLU:OE1     | 1.78                     | 1.00              |
| 18:B:676:ASP:O      | 18:B:678:PRO:HD3     | 1.60                     | 1.00              |
| 18:B:690:TRP:HE3    | 18:B:739:VAL:HG21    | 1.00                     | 1.00              |
| 18:B:1156:GLN:HA    | 18:B:1382:LYS:HZ1    | 0.83                     | 1.00              |
| 18:B:1768:ILE:HG22  | 18:B:1770:THR:CG2    | 1.89                     | 1.00              |
| 10:C32:390:HIS:HB3  | 10:C32:452:LEU:HB2   | 1.43                     | 1.00              |
| 12:A48:215:ASN:OD1  | 12:A48:592:GLN:NE2   | 1.94                     | 1.00              |
| 12:A48:560:MET:HE2  | 12:A48:615:GLN:HE22  | 1.24                     | 1.00              |
| 1:R:1424:LYS:NZ     | 6:O:105:ASN:HD21     | 1.42                     | 1.00              |
| 11:A24:6:GLU:OE1    | 21:H8:332:GLU:OE1    | 1.78                     | 1.00              |
| 11:A40:6:GLU:OE1    | 21:H16:332:GLU:OE1   | 1.78                     | 1.00              |
| 11:A16:122:LYS:HE3  | 18:B:1757:GLU:OE1    | 1.56                     | 1.00              |
| 11:A32:154:ILE:HD11 | 18:B8:1842:VAL:HG13  | 1.41                     | 1.00              |
| 23:J32:686:MET:CE   | 23:J32:694:ARG:CZ    | 2.40                     | 1.00              |
| 10:C32:453:LEU:HD13 | 10:C32:486:LEU:HD21  | 1.39                     | 1.00              |
| 8:L:1041:SER:HB3    | 8:L:1054:HIS:CE1     | 1.97                     | 1.00              |
| 8:L8:1074:ARG:CB    | 9:K8:1089:LYS:HE2    | 1.92                     | 1.00              |
| 9:K:1249:MET:HG2    | 9:K:1254:PHE:CE1     | 1.96                     | 1.00              |
| 10:C24:1757:GLN:OE1 | 11:A40:136:LEU:HD21  | 1.62                     | 1.00              |
| 10:C:1161:PHE:O     | 10:C:1164:VAL:HG23   | 1.61                     | 1.00              |
| 21:H16:285:THR:CA   | 23:J16:650:GLN:HE22  | 1.74                     | 1.00              |
| 21:H16:322:LEU:HD13 | 23:J16:689:LEU:HD23  | 1.43                     | 1.00              |
| 7:Q8:327:LEU:HD11   | 7:Q8:358:PHE:CE1     | 1.97                     | 1.00              |
| 9:K8:923:ILE:CG2    | 9:K8:929:ARG:HE      | 1.75                     | 1.00              |
| 11:A24:212:LYS:HE2  | 11:A24:585:MET:CE    | 1.77                     | 1.00              |
| 14:W:554:LYS:HD2    | 14:W:597:ARG:NH2     | 1.76                     | 1.00              |
| 14:W:746:THR:CG2    | 15:J:675:ASN:ND2     | 2.25                     | 1.00              |
| 10:C:847:ARG:HD2    | 10:C:911:ILE:CD1     | 1.89                     | 1.00              |
| 10:C8:1161:PHE:O    | 10:C8:1164:VAL:HG23  | 1.61                     | 1.00              |
| 11:A32:121:GLN:HE22 | 18:B8:1559:ALA:CA    | 1.75                     | 1.00              |
| 10:C32:390:HIS:ND1  | 10:C32:452:LEU:CD1   | 2.24                     | 1.00              |
| 10:C32:1161:PHE:O   | 10:C32:1164:VAL:HG23 | 1.61                     | 1.00              |
| 1:R:765:ASP:OD1     | 24:D:1361:ALA:HB1    | 1.60                     | 1.00              |
| 1:R:1139:ARG:HD3    | 1:R:1157:ARG:HH22    | 1.26                     | 1.00              |
| 2:M16:231:ARG:CG    | 2:M16:299:GLY:HA3    | 1.91                     | 1.00              |
| 2:M16:345:ASP:C     | 2:M16:347:LYS:H      | 1.70                     | 1.00              |
| 11:A24:215:ASN:OD1  | 11:A24:592:GLN:NE2   | 1.94                     | 1.00              |
| 11:A40:215:ASN:OD1  | 11:A40:592:GLN:NE2   | 1.94                     | 1.00              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:212:LYS:HE2   | 11:A32:585:MET:CE    | 1.77                     | 1.00              |
| 20:E8:432:ILE:HD13   | 24:D40:72:GLU:OE1    | 1.60                     | 1.00              |
| 21:H:285:THR:CA      | 23:J32:650:GLN:HE22  | 1.74                     | 1.00              |
| 1:R:1449:TRP:CZ2     | 2:M:161:ASP:O        | 2.14                     | 0.99              |
| 6:O:119:ARG:HH21     | 6:O:182:GLU:HA       | 1.26                     | 0.99              |
| 8:L8:1089:MET:HE3    | 9:K8:1000:SER:HB2    | 1.40                     | 0.99              |
| 10:C24:1548:ILE:CG1  | 24:D24:1407:PHE:HE2  | 1.75                     | 0.99              |
| 13:V:815:TYR:OH      | 15:J:627:ILE:HD11    | 1.60                     | 0.99              |
| 14:W:645:HIS:CE1     | 14:W:649:LEU:CD1     | 2.45                     | 0.99              |
| 10:C:620:PRO:HB3     | 10:C:636:VAL:HG12    | 1.44                     | 0.99              |
| 10:C:667:ILE:HG23    | 10:C:670:GLU:N       | 1.76                     | 0.99              |
| 10:C8:1757:GLN:OE1   | 16:A8:136:LEU:HD21   | 1.62                     | 0.99              |
| 18:B:410:GLN:NE2     | 18:B:538:ARG:NH2     | 2.10                     | 0.99              |
| 24:D:1:MET:HB2       | 24:D:882:GLU:OE2     | 1.60                     | 0.99              |
| 24:D32:1109:LEU:HD22 | 24:D32:1156:SER:HB2  | 1.43                     | 0.99              |
| 10:C32:679:ARG:NH2   | 10:C32:690:LEU:CD2   | 2.25                     | 0.99              |
| 10:C32:1303:LEU:HD13 | 10:C32:1323:LEU:HD23 | 1.44                     | 0.99              |
| 7:Q16:327:LEU:HD11   | 7:Q16:358:PHE:CE1    | 1.97                     | 0.99              |
| 9:K:919:MET:SD       | 9:K:938:PHE:CE2      | 2.56                     | 0.99              |
| 18:B:817:CYS:HB3     | 18:B:885:ARG:NH1     | 1.77                     | 0.99              |
| 20:E:353:ILE:CD1     | 20:E:413:PHE:HA      | 1.91                     | 0.99              |
| 10:C32:407:LYS:HD2   | 10:C32:465:PHE:CZ    | 1.97                     | 0.99              |
| 1:R:983:ARG:HH22     | 24:D:1366:PRO:HD3    | 0.90                     | 0.99              |
| 5:P:16:PHE:HE2       | 5:P:461:HIS:CE1      | 1.80                     | 0.99              |
| 8:L8:608:PHE:CZ      | 8:L8:635:MET:HA      | 1.97                     | 0.99              |
| 9:K8:1074:ARG:HD2    | 9:K8:1126:LEU:CD2    | 1.90                     | 0.99              |
| 11:A24:691:ALA:CB    | 24:D8:1397:THR:HG21  | 1.92                     | 0.99              |
| 12:A:136:LEU:HD21    | 10:C:1757:GLN:OE1    | 1.62                     | 0.99              |
| 10:C8:1549:VAL:HG13  | 10:C8:1592:VAL:HG13  | 1.42                     | 0.99              |
| 19:48:189:LEU:HD22   | 19:48:203:LEU:CD2    | 1.91                     | 0.99              |
| 1:R16:1445:GLU:OE2   | 2:M16:185:ARG:NH2    | 1.94                     | 0.99              |
| 2:M16:417:ARG:HB3    | 8:L16:298:PHE:HE2    | 0.83                     | 0.99              |
| 10:C16:847:ARG:NH2   | 10:C16:910:SER:HB2   | 1.75                     | 0.99              |
| 10:C24:407:LYS:HD2   | 10:C24:465:PHE:CZ    | 1.97                     | 0.99              |
| 11:A40:748:GLU:HB3   | 24:D24:1398:ARG:NH1  | 1.52                     | 0.99              |
| 12:A:642:GLY:HA2     | 12:A:685:ARG:CZ      | 1.88                     | 0.99              |
| 14:W:586:ILE:HD11    | 15:J:572:ASP:CG      | 1.86                     | 0.99              |
| 11:A16:121:GLN:HE22  | 18:B:1559:ALA:CA     | 1.75                     | 0.99              |
| 11:A32:215:ASN:OD1   | 11:A32:592:GLN:NE2   | 1.94                     | 0.99              |
| 18:B:536:ILE:CG2     | 18:B:545:VAL:HG11    | 1.92                     | 0.99              |
| 18:B:1256:THR:HG21   | 24:D16:1238:GLU:HG3  | 1.43                     | 0.99              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1256:THR:HG23  | 24:D32:1238:GLU:HG3  | 1.38                     | 0.99              |
| 24:D8:857:THR:HG21   | 24:D8:885:TYR:OH     | 1.60                     | 0.99              |
| 5:P16:16:PHE:HE2     | 5:P16:461:HIS:CE1    | 1.80                     | 0.99              |
| 9:K8:649:MET:HB3     | 9:K8:704:ARG:HH21    | 1.01                     | 0.99              |
| 18:B:1110:LEU:HD22   | 21:H:326:GLY:H       | 0.90                     | 0.99              |
| 19:4:189:LEU:HD22    | 19:4:203:LEU:CD2     | 1.91                     | 0.99              |
| 19:48:282:GLU:OE1    | 19:48:285:THR:OG1    | 1.79                     | 0.99              |
| 1:R8:1139:ARG:HH21   | 1:R8:1161:LEU:HD11   | 1.24                     | 0.99              |
| 6:O8:173:VAL:HG22    | 6:O8:189:LEU:HD13    | 1.44                     | 0.99              |
| 8:L:1089:MET:HG2     | 9:K:1000:SER:HB3     | 1.44                     | 0.99              |
| 11:A40:560:MET:HE2   | 11:A40:615:GLN:HE22  | 1.25                     | 0.99              |
| 10:C8:1328:PHE:HZ    | 10:C8:1377:ILE:HD11  | 1.27                     | 0.99              |
| 11:A16:714:GLY:CA    | 24:D16:1398:ARG:NH2  | 2.25                     | 0.99              |
| 21:H:291:VAL:HG12    | 23:J32:657:GLU:CG    | 1.92                     | 0.99              |
| 12:A48:212:LYS:HE2   | 12:A48:585:MET:CE    | 1.77                     | 0.99              |
| 1:R:1269:LEU:CD1     | 5:P:684:ARG:CG       | 2.41                     | 0.99              |
| 2:M16:414:GLY:CA     | 8:L16:401:LYS:NZ     | 2.25                     | 0.99              |
| 9:K:923:ILE:CG2      | 9:K:929:ARG:HE       | 1.75                     | 0.99              |
| 9:K16:894:LYS:HZ2    | 9:K16:1057:GLU:CB    | 1.72                     | 0.99              |
| 10:C24:453:LEU:HD13  | 10:C24:486:LEU:HD21  | 1.39                     | 0.99              |
| 12:A:560:MET:HE1     | 12:A:615:GLN:NE2     | 1.71                     | 0.99              |
| 10:C:679:ARG:NH2     | 10:C:690:LEU:CD2     | 2.25                     | 0.99              |
| 11:A16:560:MET:HE2   | 11:A16:615:GLN:HE22  | 1.24                     | 0.99              |
| 11:A16:706:SER:HB2   | 24:D16:1398:ARG:CD   | 1.92                     | 0.99              |
| 18:B:94:LEU:HD21     | 18:B:132:LEU:CD2     | 1.91                     | 0.99              |
| 18:B8:817:CYS:HB3    | 18:B8:885:ARG:NH1    | 1.77                     | 0.99              |
| 20:E8:353:ILE:CG2    | 20:E8:413:PHE:CE2    | 2.45                     | 0.99              |
| 21:H8:291:VAL:HG12   | 23:J8:657:GLU:CG     | 1.92                     | 0.99              |
| 23:J8:686:MET:CE     | 23:J8:694:ARG:CZ     | 2.40                     | 0.99              |
| 10:C32:1050:HIS:CD2  | 10:C32:1086:LYS:HZ2  | 1.81                     | 0.99              |
| 1:R8:1265:PHE:CZ     | 1:R8:1269:LEU:HD11   | 1.96                     | 0.99              |
| 9:K8:1249:MET:HG2    | 9:K8:1254:PHE:CE1    | 1.97                     | 0.99              |
| 10:C16:390:HIS:CG    | 10:C16:452:LEU:HB3   | 1.97                     | 0.99              |
| 10:C16:1328:PHE:HZ   | 10:C16:1377:ILE:HD11 | 1.27                     | 0.99              |
| 14:W:715:ASP:OD1     | 10:C8:1568:ARG:CG    | 2.11                     | 0.99              |
| 10:C:1348:LEU:HD13   | 10:C:1359:ILE:HD11   | 1.00                     | 0.99              |
| 10:C32:1348:LEU:HD13 | 10:C32:1359:ILE:HD11 | 1.00                     | 0.99              |
| 10:C32:1757:GLN:OE1  | 12:A48:136:LEU:HD21  | 1.62                     | 0.99              |
| 1:R8:982:GLU:CD      | 24:D40:1436:ARG:HB3  | 1.88                     | 0.99              |
| 1:R8:982:GLU:HG3     | 24:D40:1436:ARG:HH21 | 1.21                     | 0.99              |
| 5:P8:267:ARG:NH2     | 5:P8:270:GLU:OE1     | 1.94                     | 0.99              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:56:ASN:HB3     | 5:P16:59:LEU:HD12    | 1.45                     | 0.99              |
| 10:C24:1547:LYS:NZ   | 24:D24:1405:GLY:H    | 1.57                     | 0.99              |
| 10:C8:667:ILE:HD13   | 10:C8:697:HIS:CE1    | 1.97                     | 0.99              |
| 11:A32:560:MET:HE1   | 11:A32:615:GLN:NE2   | 1.71                     | 0.99              |
| 18:B:928:ARG:HH22    | 18:B:970:SER:HA      | 1.25                     | 0.99              |
| 18:B8:536:ILE:CG2    | 18:B8:545:VAL:HG11   | 1.92                     | 0.99              |
| 18:B8:1112:LYS:HE3   | 21:H24:327:SER:CA    | 1.93                     | 0.99              |
| 20:E8:345:LEU:HD21   | 24:D40:123:ALA:CB    | 1.93                     | 0.99              |
| 21:H24:285:THR:CA    | 23:J24:650:GLN:HE22  | 1.74                     | 0.99              |
| 23:J24:686:MET:CE    | 23:J24:694:ARG:CZ    | 2.40                     | 0.99              |
| 10:C32:453:LEU:CD2   | 10:C32:459:LEU:CD2   | 2.15                     | 0.99              |
| 3:N:158:TRP:CD2      | 3:N:179:LEU:HD21     | 1.98                     | 0.99              |
| 5:P8:55:ARG:NH1      | 5:P8:64:ASP:CB       | 2.26                     | 0.99              |
| 6:O8:119:ARG:HH21    | 6:O8:182:GLU:HA      | 1.26                     | 0.99              |
| 10:C24:619:LEU:HB3   | 10:C24:620:PRO:HD2   | 1.42                     | 0.99              |
| 1:R:983:ARG:HH22     | 24:D:1366:PRO:CD     | 1.75                     | 0.98              |
| 2:M8:345:ASP:C       | 2:M8:347:LYS:H       | 1.70                     | 0.98              |
| 9:K:614:PHE:C        | 9:K:683:GLN:NE2      | 2.20                     | 0.98              |
| 10:C24:847:ARG:NH2   | 10:C24:910:SER:HB2   | 1.75                     | 0.98              |
| 10:C8:1348:LEU:HD13  | 10:C8:1359:ILE:HD11  | 1.00                     | 0.98              |
| 11:A32:386:GLY:O     | 11:A32:459:ARG:NH1   | 1.96                     | 0.98              |
| 18:B8:1900:ILE:CD1   | 18:B8:1946:LEU:HD22  | 1.93                     | 0.98              |
| 20:E:353:ILE:CG2     | 20:E:413:PHE:CE2     | 2.45                     | 0.98              |
| 2:M:345:ASP:C        | 2:M:347:LYS:H        | 1.70                     | 0.98              |
| 3:N:4:GLN:HE22       | 3:N:44:GLY:C         | 1.71                     | 0.98              |
| 2:M8:202:LYS:HZ1     | 2:M8:208:SER:N       | 1.61                     | 0.98              |
| 2:M16:414:GLY:HA2    | 8:L16:401:LYS:HZ2    | 0.84                     | 0.98              |
| 5:P16:101:LEU:HD22   | 5:P16:133:TYR:CZ     | 1.87                     | 0.98              |
| 9:K8:716:ALA:CB      | 10:C32:503:THR:HB    | 1.92                     | 0.98              |
| 10:C:1549:VAL:HG13   | 10:C:1592:VAL:HG13   | 1.42                     | 0.98              |
| 11:A16:91:GLU:HB3    | 18:B:1112:LYS:NZ     | 1.46                     | 0.98              |
| 18:B:609:TYR:HD2     | 18:B:610:VAL:HG22    | 1.25                     | 0.98              |
| 21:H16:291:VAL:HG12  | 23:J16:657:GLU:CG    | 1.92                     | 0.98              |
| 21:H16:312:GLN:HG2   | 21:H16:316:ILE:HD12  | 1.46                     | 0.98              |
| 10:C32:1703:ILE:HD12 | 10:C32:1741:MET:CE   | 1.93                     | 0.98              |
| 5:P:56:ASN:HB3       | 5:P:59:LEU:HD12      | 1.45                     | 0.98              |
| 5:P:220:GLU:OE2      | 5:P:232:ARG:NH1      | 1.95                     | 0.98              |
| 8:L8:270:LEU:HD22    | 12:A48:155:SER:HB2   | 1.41                     | 0.98              |
| 10:C16:1757:GLN:OE1  | 11:A24:136:LEU:HD21  | 1.62                     | 0.98              |
| 11:A24:737:GLU:HG3   | 24:D16:871:ARG:HH21  | 0.84                     | 0.98              |
| 10:C24:1348:LEU:HD13 | 10:C24:1359:ILE:HD11 | 1.00                     | 0.98              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A40:386:GLY:O     | 11:A40:459:ARG:NH1   | 1.96                     | 0.98              |
| 10:C:619:LEU:HB3     | 10:C:620:PRO:HD2     | 1.42                     | 0.98              |
| 11:A32:560:MET:HE2   | 11:A32:615:GLN:HE22  | 1.25                     | 0.98              |
| 18:B:1900:ILE:CD1    | 18:B:1946:LEU:HD22   | 1.93                     | 0.98              |
| 18:B8:685:SER:C      | 18:B8:687:SER:H      | 1.71                     | 0.98              |
| 21:H24:312:GLN:HG2   | 21:H24:316:ILE:HD11  | 0.99                     | 0.98              |
| 21:H24:322:LEU:HD13  | 23:J24:689:LEU:HD23  | 1.43                     | 0.98              |
| 10:C32:667:ILE:CD1   | 10:C32:700:MET:CE    | 2.40                     | 0.98              |
| 1:R8:1265:PHE:CE2    | 5:P8:684:ARG:HD3     | 1.93                     | 0.98              |
| 3:N16:4:GLN:HE22     | 3:N16:44:GLY:C       | 1.71                     | 0.98              |
| 5:P8:56:ASN:HB3      | 5:P8:59:LEU:HD12     | 1.45                     | 0.98              |
| 5:P8:220:GLU:OE2     | 5:P8:232:ARG:NH1     | 1.95                     | 0.98              |
| 9:K:1085:TYR:HH      | 9:K:1093:SER:HA      | 1.21                     | 0.98              |
| 9:K8:1039:ASP:OD1    | 9:K8:1096:LYS:NZ     | 1.94                     | 0.98              |
| 10:C16:572:ILE:HD11  | 10:C16:606:MET:HE2   | 0.99                     | 0.98              |
| 18:B8:609:TYR:HD2    | 18:B8:610:VAL:CG2    | 1.77                     | 0.98              |
| 1:R8:982:GLU:OE1     | 24:D40:1436:ARG:CG   | 2.11                     | 0.98              |
| 5:P16:220:GLU:OE2    | 5:P16:232:ARG:NH1    | 1.95                     | 0.98              |
| 9:K8:581:ASP:HB3     | 9:K8:625:ARG:HH22    | 0.82                     | 0.98              |
| 10:C16:1348:LEU:HD13 | 10:C16:1359:ILE:HD11 | 1.00                     | 0.98              |
| 10:C24:1814:LYS:CE   | 23:J24:738:MET:SD    | 2.51                     | 0.98              |
| 10:C:667:ILE:HD13    | 10:C:697:HIS:CE1     | 1.94                     | 0.98              |
| 10:C8:1703:ILE:HD12  | 10:C8:1741:MET:CE    | 1.93                     | 0.98              |
| 21:H:231:HIS:CD2     | 23:J32:596:GLN:HE22  | 1.76                     | 0.98              |
| 21:H:312:GLN:HG2     | 21:H:316:ILE:HD12    | 1.46                     | 0.98              |
| 23:J16:686:MET:CE    | 23:J16:694:ARG:CZ    | 2.40                     | 0.98              |
| 2:M16:672:TYR:HB3    | 2:M16:680:LYS:HD2    | 1.00                     | 0.98              |
| 5:P16:55:ARG:NH1     | 5:P16:64:ASP:CB      | 2.26                     | 0.98              |
| 10:C24:407:LYS:HG3   | 10:C24:465:PHE:CE1   | 1.99                     | 0.98              |
| 10:C8:572:ILE:HD11   | 10:C8:606:MET:HE2    | 0.99                     | 0.98              |
| 10:C8:619:LEU:HB3    | 10:C8:620:PRO:HD2    | 1.42                     | 0.98              |
| 11:A16:676:TYR:OH    | 24:D16:1395:SER:N    | 1.96                     | 0.98              |
| 18:B:1112:LYS:HE3    | 21:H:327:SER:HA      | 1.45                     | 0.98              |
| 18:B8:786:ASP:OD1    | 24:D32:1066:VAL:HG11 | 1.60                     | 0.98              |
| 1:R:1424:LYS:HZ2     | 6:O:105:ASN:ND2      | 1.40                     | 0.98              |
| 5:P:179:TYR:HE1      | 5:P:437:GLY:HA3      | 0.85                     | 0.98              |
| 8:L8:608:PHE:CE2     | 8:L8:635:MET:HB3     | 1.97                     | 0.98              |
| 8:L8:1041:SER:HB3    | 8:L8:1054:HIS:CE1    | 1.97                     | 0.98              |
| 9:K:792:LEU:HD12     | 9:K:864:ILE:HD11     | 1.00                     | 0.98              |
| 10:C8:1050:HIS:NE2   | 10:C8:1086:LYS:NZ    | 2.12                     | 0.98              |
| 11:A16:676:TYR:CE2   | 24:D16:1395:SER:CB   | 2.47                     | 0.98              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:191:PHE:CE2     | 18:B:193:LYS:HA      | 1.98                     | 0.98              |
| 18:B8:690:TRP:HE3    | 18:B8:739:VAL:HG21   | 1.00                     | 0.98              |
| 21:H8:312:GLN:NE2    | 22:I8:290:ASP:OD2    | 1.97                     | 0.98              |
| 21:H16:312:GLN:NE2   | 22:I16:290:ASP:OD2   | 1.97                     | 0.98              |
| 24:D:403:ARG:NE      | 24:D16:744:LEU:O     | 1.96                     | 0.98              |
| 10:C32:1626:GLN:HE21 | 10:C32:1692:LYS:HZ3  | 1.09                     | 0.98              |
| 2:M:377:ARG:HH12     | 2:M:477:ASP:CB       | 1.75                     | 0.98              |
| 5:P:267:ARG:NH2      | 5:P:270:GLU:OE1      | 1.94                     | 0.98              |
| 6:O:176:ASN:HD21     | 6:O:179:LYS:HE3      | 1.24                     | 0.98              |
| 10:C24:1161:PHE:O    | 10:C24:1164:VAL:HG23 | 1.61                     | 0.98              |
| 12:A:386:GLY:O       | 12:A:459:ARG:NH1     | 1.96                     | 0.98              |
| 14:W:659:ARG:NH2     | 15:J:583:LEU:HD23    | 1.78                     | 0.98              |
| 14:W:715:ASP:OD1     | 10:C8:1568:ARG:HG2   | 1.63                     | 0.98              |
| 10:C:572:ILE:HD11    | 10:C:606:MET:HE2     | 0.99                     | 0.98              |
| 10:C:1703:ILE:HD12   | 10:C:1741:MET:CE     | 1.93                     | 0.98              |
| 18:B:729:LEU:HB2     | 18:B:1196:MET:HE1    | 1.46                     | 0.98              |
| 18:B8:410:GLN:NE2    | 18:B8:538:ARG:NH2    | 2.10                     | 0.98              |
| 1:R:1078:SER:CB      | 5:P:713:LEU:HD21     | 1.94                     | 0.98              |
| 3:N8:158:TRP:CD2     | 3:N8:179:LEU:HD21    | 1.98                     | 0.98              |
| 5:P:607:PHE:CD1      | 5:P:633:LEU:HD12     | 1.97                     | 0.98              |
| 9:K8:635:ALA:HB2     | 9:K8:655:GLN:OE1     | 1.63                     | 0.98              |
| 10:C16:1161:PHE:O    | 10:C16:1164:VAL:HG23 | 1.61                     | 0.98              |
| 10:C16:1303:LEU:HD13 | 10:C16:1323:LEU:HD23 | 1.44                     | 0.98              |
| 11:A24:386:GLY:O     | 11:A24:459:ARG:NH1   | 1.96                     | 0.98              |
| 11:A40:465:SER:HB3   | 24:D32:1100:GLN:HE22 | 1.24                     | 0.98              |
| 13:V:745:LEU:HD11    | 15:J:557:ARG:NH1     | 1.78                     | 0.98              |
| 10:C:153:ALA:HB1     | 24:D:1403:LEU:HD11   | 1.42                     | 0.98              |
| 10:C8:620:PRO:HB3    | 10:C8:636:VAL:HG12   | 1.44                     | 0.98              |
| 11:A16:386:GLY:O     | 11:A16:459:ARG:NH1   | 1.96                     | 0.98              |
| 20:E:344:PRO:O       | 24:D:121:GLU:OE1     | 1.82                     | 0.98              |
| 2:M16:627:TYR:H      | 2:M16:627:TYR:HD2    | 1.03                     | 0.98              |
| 3:N16:158:TRP:CD2    | 3:N16:179:LEU:HD21   | 1.98                     | 0.98              |
| 9:K8:614:PHE:C       | 9:K8:683:GLN:NE2     | 2.20                     | 0.98              |
| 9:K8:1085:TYR:CZ     | 9:K8:1093:SER:CA     | 2.47                     | 0.98              |
| 10:C16:1547:LYS:NZ   | 24:D8:1405:GLY:N     | 2.09                     | 0.98              |
| 10:C24:578:LEU:O     | 10:C24:584:ILE:CD1   | 2.12                     | 0.98              |
| 10:C24:1703:ILE:HD12 | 10:C24:1741:MET:CE   | 1.93                     | 0.98              |
| 24:D:1385:MET:SD     | 24:D:1464:PHE:HE1    | 1.81                     | 0.98              |
| 9:K:581:ASP:HB3      | 9:K:625:ARG:HH22     | 0.82                     | 0.97              |
| 9:K8:631:VAL:HG12    | 9:K8:764:VAL:HB      | 1.46                     | 0.97              |
| 10:C24:572:ILE:HD11  | 10:C24:606:MET:HE2   | 0.99                     | 0.97              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1328:PHE:HZ  | 10:C24:1377:ILE:HD11 | 1.27                     | 0.97              |
| 14:W:739:ARG:HH22   | 15:J:664:GLN:NE2     | 1.59                     | 0.97              |
| 11:A32:154:ILE:HD12 | 18:B8:1842:VAL:HG13  | 1.45                     | 0.97              |
| 18:B8:152:HIS:HB3   | 18:B8:163:ILE:HD13   | 1.46                     | 0.97              |
| 18:B8:1156:GLN:HA   | 18:B8:1382:LYS:HZ1   | 0.83                     | 0.97              |
| 21:H:312:GLN:NE2    | 22:I:290:ASP:OD2     | 1.97                     | 0.97              |
| 21:H16:312:GLN:HG2  | 21:H16:316:ILE:HD11  | 0.99                     | 0.97              |
| 24:D:400:VAL:HG11   | 24:D16:751:MET:HB3   | 1.42                     | 0.97              |
| 10:C32:1271:PHE:CE2 | 10:C32:1284:ASP:CB   | 2.47                     | 0.97              |
| 12:A48:386:GLY:O    | 12:A48:459:ARG:NH1   | 1.96                     | 0.97              |
| 6:O8:119:ARG:NH2    | 6:O8:182:GLU:HA      | 1.79                     | 0.97              |
| 7:Q16:92:GLY:O      | 7:Q16:94:SER:N       | 1.97                     | 0.97              |
| 8:L16:1069:LEU:CD2  | 9:K16:1086:VAL:HG11  | 1.94                     | 0.97              |
| 10:C16:407:LYS:HG3  | 10:C16:465:PHE:CE1   | 1.98                     | 0.97              |
| 10:C8:593:ARG:NH1   | 10:C8:655:SER:OG     | 1.98                     | 0.97              |
| 10:C8:667:ILE:O     | 10:C8:668:ALA:C      | 1.68                     | 0.97              |
| 18:B:152:HIS:HB3    | 18:B:163:ILE:HD13    | 1.46                     | 0.97              |
| 18:B:349:PHE:CE1    | 18:B:353:ILE:CD1     | 2.47                     | 0.97              |
| 18:B:685:SER:C      | 18:B:687:SER:H       | 1.71                     | 0.97              |
| 18:B8:191:PHE:CE2   | 18:B8:193:LYS:HA     | 1.99                     | 0.97              |
| 18:B8:1110:LEU:HD22 | 21:H24:326:GLY:H     | 0.82                     | 0.97              |
| 10:C32:578:LEU:O    | 10:C32:584:ILE:CD1   | 2.12                     | 0.97              |
| 10:C32:1050:HIS:NE2 | 10:C32:1086:LYS:NZ   | 2.12                     | 0.97              |
| 5:P:607:PHE:CE1     | 5:P:633:LEU:HD13     | 1.98                     | 0.97              |
| 10:C:1303:LEU:HD13  | 10:C:1323:LEU:HD23   | 1.44                     | 0.97              |
| 11:A16:90:PHE:C     | 18:B:1800:ARG:NH2    | 2.23                     | 0.97              |
| 11:A32:212:LYS:HE3  | 11:A32:585:MET:HE1   | 1.27                     | 0.97              |
| 18:B8:1529:GLU:CD   | 24:D32:1415:LEU:CD1  | 2.35                     | 0.97              |
| 21:H8:312:GLN:HG2   | 21:H8:316:ILE:HD11   | 0.99                     | 0.97              |
| 21:H24:312:GLN:NE2  | 22:I24:290:ASP:OD2   | 1.97                     | 0.97              |
| 10:C32:278:ARG:NH1  | 10:C32:287:SER:HB2   | 1.78                     | 0.97              |
| 7:Q:297:VAL:HG13    | 7:Q:301:ARG:HD2      | 1.46                     | 0.97              |
| 5:P8:614:VAL:N      | 5:P8:629:ARG:HH22    | 1.62                     | 0.97              |
| 10:C24:1687:GLU:OE2 | 10:C24:1806:ARG:NH2  | 1.97                     | 0.97              |
| 10:C:593:ARG:NH1    | 10:C:655:SER:OG      | 1.98                     | 0.97              |
| 11:A32:24:ALA:O     | 23:J24:705:TRP:CE2   | 2.18                     | 0.97              |
| 18:B:1940:ALA:CB    | 18:B:1950:ILE:CD1    | 2.42                     | 0.97              |
| 18:B8:1940:ALA:CB   | 18:B8:1950:ILE:CD1   | 2.42                     | 0.97              |
| 10:C32:572:ILE:HD11 | 10:C32:606:MET:HE2   | 0.99                     | 0.97              |
| 10:C32:1328:PHE:HZ  | 10:C32:1377:ILE:HD11 | 1.27                     | 0.97              |
| 2:M:185:ARG:HH11    | 2:M:213:LEU:HD11     | 1.29                     | 0.97              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P:401:ARG:HD2      | 5:P:414:VAL:HG21    | 1.00                     | 0.97              |
| 9:K:869:GLU:OE1      | 9:K:944:ASN:HB3     | 1.63                     | 0.97              |
| 10:C16:278:ARG:NH1   | 10:C16:287:SER:HB2  | 1.78                     | 0.97              |
| 10:C16:1453:ARG:HH22 | 24:D8:1150:GLY:HA2  | 1.27                     | 0.97              |
| 10:C24:390:HIS:CD2   | 10:C24:449:GLU:OE2  | 2.17                     | 0.97              |
| 10:C:278:ARG:NH1     | 10:C:287:SER:HB2    | 1.78                     | 0.97              |
| 18:B:750:GLU:HG3     | 18:B:760:ARG:CZ     | 1.94                     | 0.97              |
| 18:B8:643:MET:HE1    | 18:B8:711:CYS:HB3   | 1.45                     | 0.97              |
| 10:C32:1625:SER:O    | 10:C32:1628:SER:OG  | 1.83                     | 0.97              |
| 5:P:152:ILE:HG21     | 14:W:762:GLN:HE21   | 1.20                     | 0.97              |
| 8:L16:1041:SER:HB3   | 8:L16:1054:HIS:CE1  | 1.97                     | 0.97              |
| 10:C24:278:ARG:NH1   | 10:C24:287:SER:HB2  | 1.78                     | 0.97              |
| 11:A40:560:MET:HE1   | 11:A40:615:GLN:NE2  | 1.72                     | 0.97              |
| 12:A:153:ARG:CB      | 10:C8:74:ASP:OD1    | 2.12                     | 0.97              |
| 12:A:560:MET:HE2     | 12:A:615:GLN:HE22   | 1.24                     | 0.97              |
| 10:C:578:LEU:O       | 10:C:584:ILE:CD1    | 2.12                     | 0.97              |
| 10:C:1328:PHE:HZ     | 10:C:1377:ILE:HD11  | 1.27                     | 0.97              |
| 18:B8:609:TYR:HD2    | 18:B8:610:VAL:HG22  | 1.25                     | 0.97              |
| 18:B8:750:GLU:HG3    | 18:B8:760:ARG:CZ    | 1.94                     | 0.97              |
| 24:D:1099:ARG:HD3    | 24:D:1149:VAL:HG11  | 1.44                     | 0.97              |
| 10:C32:1687:GLU:OE2  | 10:C32:1806:ARG:NH2 | 1.97                     | 0.97              |
| 2:M8:377:ARG:HH12    | 2:M8:477:ASP:CB     | 1.75                     | 0.97              |
| 7:Q:92:GLY:O         | 7:Q:94:SER:N        | 1.97                     | 0.97              |
| 5:P8:16:PHE:HE2      | 5:P8:461:HIS:CE1    | 1.80                     | 0.97              |
| 5:P8:101:LEU:HD23    | 5:P8:133:TYR:CE1    | 1.99                     | 0.97              |
| 6:O16:119:ARG:HH21   | 6:O16:182:GLU:HA    | 1.26                     | 0.97              |
| 10:C16:593:ARG:NH1   | 10:C16:655:SER:OG   | 1.98                     | 0.97              |
| 11:A24:468:VAL:CG2   | 24:D16:1100:GLN:OE1 | 2.11                     | 0.97              |
| 10:C24:593:ARG:NH1   | 10:C24:655:SER:OG   | 1.98                     | 0.97              |
| 10:C8:278:ARG:NH1    | 10:C8:287:SER:HB2   | 1.78                     | 0.97              |
| 11:A32:698:LYS:HE2   | 24:D32:1393:GLY:HA2 | 1.46                     | 0.97              |
| 18:B8:112:GLU:CD     | 18:B8:130:MET:SD    | 2.48                     | 0.97              |
| 18:B8:195:MET:CE     | 18:B8:199:LEU:CD2   | 2.18                     | 0.97              |
| 24:D32:749:ARG:NH2   | 24:D40:397:ALA:H    | 1.61                     | 0.97              |
| 12:A48:560:MET:HE1   | 12:A48:615:GLN:NE2  | 1.72                     | 0.97              |
| 2:M:417:ARG:NH1      | 8:L:298:PHE:O       | 1.97                     | 0.97              |
| 5:P:402:LEU:HD13     | 5:P:433:LEU:HB3     | 0.97                     | 0.97              |
| 10:C16:1074:LEU:CD1  | 10:C16:1075:ASP:CA  | 2.33                     | 0.97              |
| 10:C16:1770:LEU:O    | 10:C16:1836:LYS:HE3 | 1.64                     | 0.97              |
| 11:A40:24:ALA:O      | 23:J16:705:TRP:CE2  | 2.18                     | 0.97              |
| 10:C8:578:LEU:O      | 10:C8:584:ILE:CD1   | 2.12                     | 0.97              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:643:MET:HE1     | 18:B:711:CYS:HB3     | 1.45                     | 0.97              |
| 18:B8:349:PHE:CE1    | 18:B8:353:ILE:CD1    | 2.47                     | 0.97              |
| 22:I8:146:SER:CB     | 23:J8:574:ARG:NH1    | 2.26                     | 0.97              |
| 1:R:1269:LEU:HD13    | 5:P:684:ARG:HG2      | 0.98                     | 0.97              |
| 5:P:55:ARG:NH1       | 5:P:64:ASP:CB        | 2.26                     | 0.97              |
| 5:P8:313:TRP:HZ2     | 5:P8:345:MET:CE      | 1.78                     | 0.97              |
| 9:K:631:VAL:HG12     | 9:K:764:VAL:HB       | 1.46                     | 0.97              |
| 9:K:1074:ARG:CZ      | 9:K:1126:LEU:HD22    | 1.94                     | 0.97              |
| 10:C8:1687:GLU:OE2   | 10:C8:1806:ARG:NH2   | 1.97                     | 0.97              |
| 11:A32:91:GLU:HB2    | 18:B8:1112:LYS:HZ1   | 1.26                     | 0.97              |
| 18:B:514:THR:CG2     | 18:B:549:TRP:CZ3     | 2.48                     | 0.97              |
| 19:48:250:ILE:HG21   | 20:E8:165:ARG:NH2    | 1.80                     | 0.97              |
| 21:H8:231:HIS:CD2    | 23:J8:596:GLN:HE22   | 1.76                     | 0.97              |
| 1:R:1428:VAL:HG21    | 6:O:165:LYS:NZ       | 1.75                     | 0.97              |
| 5:P:214:LEU:HD23     | 5:P:236:VAL:HG11     | 1.46                     | 0.97              |
| 5:P16:313:TRP:HZ2    | 5:P16:345:MET:CE     | 1.78                     | 0.97              |
| 10:C16:578:LEU:O     | 10:C16:584:ILE:CD1   | 2.12                     | 0.97              |
| 11:A40:474:LEU:HD11  | 24:D32:1099:ARG:HH22 | 1.30                     | 0.97              |
| 10:C:1770:LEU:O      | 10:C:1836:LYS:HE3    | 1.64                     | 0.97              |
| 11:A16:703:ALA:HB1   | 24:D16:1398:ARG:HH11 | 1.29                     | 0.97              |
| 18:B8:514:THR:CG2    | 18:B8:549:TRP:CZ3    | 2.48                     | 0.97              |
| 10:C32:407:LYS:HG3   | 10:C32:465:PHE:CE1   | 1.98                     | 0.97              |
| 1:R:983:ARG:O        | 24:D:1360:ALA:HB2    | 1.65                     | 0.96              |
| 2:M:202:LYS:HZ1      | 2:M:208:SER:N        | 1.63                     | 0.96              |
| 2:M:844:VAL:HG22     | 4:T:660:LEU:HD11     | 1.47                     | 0.96              |
| 5:P:251:LYS:NZ       | 14:W:765:LYS:HZ3     | 1.63                     | 0.96              |
| 5:P8:214:LEU:HD23    | 5:P8:236:VAL:HG11    | 1.46                     | 0.96              |
| 9:K8:634:LEU:HD22    | 9:K8:754:ARG:NH1     | 1.80                     | 0.96              |
| 9:K8:955:TYR:CZ      | 9:K8:985:PHE:N       | 2.33                     | 0.96              |
| 9:K8:1074:ARG:CZ     | 9:K8:1126:LEU:HD22   | 1.94                     | 0.96              |
| 10:C16:1703:ILE:HD12 | 10:C16:1741:MET:CE   | 1.93                     | 0.96              |
| 11:A24:24:ALA:O      | 23:J8:705:TRP:CE2    | 2.18                     | 0.96              |
| 10:C24:667:ILE:HD13  | 10:C24:697:HIS:CE1   | 1.94                     | 0.96              |
| 10:C8:556:VAL:HG13   | 10:C8:565:ARG:HH22   | 1.27                     | 0.96              |
| 11:A16:24:ALA:O      | 23:J32:705:TRP:CE2   | 2.18                     | 0.96              |
| 18:B:609:TYR:HD2     | 18:B:610:VAL:CG2     | 1.76                     | 0.96              |
| 18:B:1110:LEU:HD22   | 21:H:326:GLY:CA      | 1.87                     | 0.96              |
| 18:B8:817:CYS:HB3    | 18:B8:885:ARG:HH12   | 1.29                     | 0.96              |
| 19:4:100:ILE:CG2     | 19:4:102:LEU:HG      | 1.95                     | 0.96              |
| 19:48:252:ARG:CG     | 19:48:281:TRP:CH2    | 2.43                     | 0.96              |
| 3:N8:4:GLN:HE22      | 3:N8:44:GLY:C        | 1.71                     | 0.96              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:O16:119:ARG:NH2    | 6:O16:182:GLU:HA     | 1.78                     | 0.96              |
| 8:L16:173:ASP:HB3    | 12:A48:783:PHE:CE1   | 2.00                     | 0.96              |
| 9:K8:581:ASP:CB      | 9:K8:625:ARG:HH22    | 1.77                     | 0.96              |
| 9:K8:751:LEU:CD2     | 9:K8:754:ARG:HH11    | 1.78                     | 0.96              |
| 10:C16:1050:HIS:NE2  | 10:C16:1086:LYS:NZ   | 2.12                     | 0.96              |
| 11:A24:747:MET:HE1   | 24:D16:167:ARG:HH12  | 1.26                     | 0.96              |
| 10:C24:1303:LEU:HD13 | 10:C24:1323:LEU:HD23 | 1.43                     | 0.96              |
| 10:C24:1547:LYS:HD3  | 24:D24:1406:SER:N    | 1.80                     | 0.96              |
| 11:A40:748:GLU:OE2   | 24:D24:1398:ARG:NH1  | 1.97                     | 0.96              |
| 18:B:32:LEU:HD13     | 18:B:163:ILE:HD12    | 1.46                     | 0.96              |
| 18:B:817:CYS:HB3     | 18:B:885:ARG:HH12    | 1.28                     | 0.96              |
| 1:R:1326:GLY:CA      | 10:C:1154:TRP:NE1    | 2.25                     | 0.96              |
| 2:M8:185:ARG:HH11    | 2:M8:213:LEU:HD11    | 1.29                     | 0.96              |
| 2:M8:428:SER:HB2     | 8:L8:355:SER:HG      | 0.82                     | 0.96              |
| 5:P:600:PHE:HE2      | 5:P:638:SER:HG       | 1.04                     | 0.96              |
| 5:P8:611:LEU:CA      | 5:P8:629:ARG:CZ      | 2.38                     | 0.96              |
| 7:Q8:92:GLY:O        | 7:Q8:94:SER:N        | 1.97                     | 0.96              |
| 7:Q16:297:VAL:HG13   | 7:Q16:301:ARG:HD2    | 1.46                     | 0.96              |
| 9:K8:869:GLU:OE1     | 9:K8:944:ASN:HB3     | 1.64                     | 0.96              |
| 10:C:1537:GLU:OE2    | 10:C8:113:LEU:HD22   | 1.63                     | 0.96              |
| 11:A16:560:MET:HE1   | 11:A16:615:GLN:NE2   | 1.71                     | 0.96              |
| 11:A32:388:VAL:H     | 11:A32:459:ARG:HH12  | 1.08                     | 0.96              |
| 18:B8:32:LEU:HD13    | 18:B8:163:ILE:HD12   | 1.46                     | 0.96              |
| 2:M16:544:LEU:CD1    | 2:M16:586:ALA:O      | 2.14                     | 0.96              |
| 3:N16:4:GLN:NE2      | 3:N16:44:GLY:O       | 1.99                     | 0.96              |
| 5:P16:101:LEU:CD2    | 5:P16:133:TYR:CE1    | 2.30                     | 0.96              |
| 6:O16:173:VAL:HG22   | 6:O16:189:LEU:HD13   | 1.44                     | 0.96              |
| 9:K:635:ALA:HB2      | 9:K:655:GLN:OE1      | 1.64                     | 0.96              |
| 10:C24:390:HIS:ND1   | 10:C24:452:LEU:HB2   | 1.79                     | 0.96              |
| 10:C24:1625:SER:O    | 10:C24:1628:SER:OG   | 1.83                     | 0.96              |
| 10:C:1050:HIS:CD2    | 10:C:1086:LYS:HZ2    | 1.77                     | 0.96              |
| 18:B:112:GLU:CD      | 18:B:130:MET:SD      | 2.48                     | 0.96              |
| 24:D:400:VAL:CG1     | 24:D16:751:MET:CB    | 2.42                     | 0.96              |
| 24:D32:749:ARG:HH22  | 24:D40:397:ALA:N     | 1.62                     | 0.96              |
| 6:O:119:ARG:NH2      | 6:O:182:GLU:HA       | 1.79                     | 0.96              |
| 11:A40:798:PHE:CE1   | 11:A40:847:ARG:CZ    | 2.48                     | 0.96              |
| 11:A16:519:MET:HE2   | 11:A16:569:MET:HE1   | 1.47                     | 0.96              |
| 11:A16:798:PHE:CE1   | 11:A16:847:ARG:CZ    | 2.48                     | 0.96              |
| 18:B8:1439:LYS:HE2   | 24:D32:1257:ASN:HB3  | 0.98                     | 0.96              |
| 2:M16:185:ARG:HH11   | 2:M16:213:LEU:HD11   | 1.29                     | 0.96              |
| 5:P:398:LYS:HB3      | 5:P:426:MET:HE2      | 1.43                     | 0.96              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:1271:PHE:CE2    | 10:C:1284:ASP:CB     | 2.47                     | 0.96              |
| 10:C8:639:MET:HE3    | 10:C8:643:LEU:CD1    | 1.95                     | 0.96              |
| 18:B:484:TYR:CE2     | 18:B:556:ILE:HD13    | 2.00                     | 0.96              |
| 18:B:664:LEU:HD11    | 18:B:729:LEU:HD21    | 1.46                     | 0.96              |
| 2:M:416:VAL:CG1      | 8:L:398:ALA:HB2      | 1.95                     | 0.96              |
| 3:N:4:GLN:NE2        | 3:N:44:GLY:O         | 1.99                     | 0.96              |
| 10:C16:407:LYS:HD2   | 10:C16:465:PHE:CZ    | 1.97                     | 0.96              |
| 10:C24:1682:VAL:HG21 | 10:C24:1758:LEU:HD23 | 1.47                     | 0.96              |
| 12:A:362:ARG:HD2     | 12:A:366:ARG:HH22    | 1.03                     | 0.96              |
| 10:C:1687:GLU:OE2    | 10:C:1806:ARG:NH2    | 1.97                     | 0.96              |
| 18:B:917:PHE:CE2     | 18:B:960:GLN:NE2     | 2.33                     | 0.96              |
| 18:B8:729:LEU:HB2    | 18:B8:1196:MET:HE1   | 1.46                     | 0.96              |
| 20:E:429:PRO:HD3     | 24:D:72:GLU:OE2      | 1.65                     | 0.96              |
| 10:C32:620:PRO:HB3   | 10:C32:636:VAL:HG12  | 1.44                     | 0.96              |
| 2:M16:377:ARG:HH12   | 2:M16:477:ASP:CB     | 1.75                     | 0.96              |
| 5:P:16:PHE:CE1       | 6:O:311:LEU:CD1      | 2.49                     | 0.96              |
| 8:L16:851:PRO:CB     | 9:K16:1283:PRO:CB    | 2.44                     | 0.96              |
| 11:A24:798:PHE:CE1   | 11:A24:847:ARG:CZ    | 2.48                     | 0.96              |
| 12:A:798:PHE:CE1     | 12:A:847:ARG:CZ      | 2.48                     | 0.96              |
| 11:A16:388:VAL:H     | 11:A16:459:ARG:HH12  | 1.08                     | 0.96              |
| 11:A32:707:LEU:CD2   | 11:A32:767:ARG:HH22  | 1.79                     | 0.96              |
| 11:A32:798:PHE:HE1   | 11:A32:847:ARG:NH1   | 1.64                     | 0.96              |
| 18:B:410:GLN:NE2     | 18:B:538:ARG:HH22    | 1.62                     | 0.96              |
| 21:H:312:GLN:HG2     | 21:H:316:ILE:HD11    | 0.99                     | 0.96              |
| 24:D:400:VAL:CB      | 24:D16:751:MET:HE2   | 1.94                     | 0.96              |
| 10:C32:1770:LEU:O    | 10:C32:1836:LYS:HE3  | 1.65                     | 0.96              |
| 12:A48:519:MET:HE2   | 12:A48:569:MET:HE1   | 1.47                     | 0.96              |
| 2:M:417:ARG:CB       | 8:L:346:TRP:CZ2      | 2.49                     | 0.96              |
| 10:C16:1271:PHE:CE2  | 10:C16:1284:ASP:CB   | 2.47                     | 0.96              |
| 10:C24:586:PRO:CD    | 10:C24:650:ARG:NH1   | 2.29                     | 0.96              |
| 12:A:519:MET:HE2     | 12:A:569:MET:HE1     | 1.47                     | 0.96              |
| 11:A16:90:PHE:CG     | 18:B:1788:ILE:HD13   | 1.99                     | 0.96              |
| 18:B:1940:ALA:HB1    | 18:B:1950:ILE:HD11   | 1.46                     | 0.96              |
| 12:A48:302:GLN:NE2   | 12:A48:324:ARG:NH1   | 2.14                     | 0.96              |
| 12:A48:798:PHE:CE1   | 12:A48:847:ARG:CZ    | 2.48                     | 0.96              |
| 1:R16:1166:ASN:ND2   | 5:P16:672:LEU:HD22   | 1.78                     | 0.96              |
| 2:M16:202:LYS:HZ1    | 2:M16:208:SER:N      | 1.62                     | 0.96              |
| 7:Q8:143:ARG:NH1     | 7:Q8:190:PRO:O       | 1.99                     | 0.96              |
| 7:Q8:297:VAL:HG13    | 7:Q8:301:ARG:HD2     | 1.46                     | 0.96              |
| 6:O16:20:SER:OG      | 6:O16:22:ASP:OD1     | 1.84                     | 0.96              |
| 7:Q16:27:GLN:NE2     | 7:Q16:33:ARG:HG2     | 1.81                     | 0.96              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:620:PRO:HB3   | 10:C16:636:VAL:HG12 | 1.44                     | 0.96              |
| 10:C24:1002:LEU:HD12 | 10:C24:1019:ARG:NH1 | 1.81                     | 0.96              |
| 11:A40:212:LYS:HE2   | 11:A40:585:MET:CE   | 1.77                     | 0.96              |
| 11:A32:798:PHE:CE1   | 11:A32:847:ARG:CZ   | 2.48                     | 0.96              |
| 18:B8:917:PHE:CE2    | 18:B8:960:GLN:NE2   | 2.33                     | 0.96              |
| 20:E:429:PRO:HG2     | 24:D:69:VAL:HG13    | 1.44                     | 0.96              |
| 19:48:100:ILE:CG2    | 19:48:102:LEU:HG    | 1.95                     | 0.96              |
| 1:R8:1466:LYS:HB3    | 6:O8:160:LEU:HD13   | 0.96                     | 0.95              |
| 10:C24:1271:PHE:CE2  | 10:C24:1284:ASP:CB  | 2.47                     | 0.95              |
| 10:C:153:ALA:HB1     | 24:D:1403:LEU:HD12  | 1.44                     | 0.95              |
| 18:B:928:ARG:NH1     | 18:B:969:ASP:O      | 1.99                     | 0.95              |
| 20:E:353:ILE:HD12    | 20:E:413:PHE:CG     | 2.00                     | 0.95              |
| 20:E8:432:ILE:HG21   | 24:D40:72:GLU:CG    | 1.94                     | 0.95              |
| 21:H24:312:GLN:HE22  | 22:I24:290:ASP:HB3  | 1.31                     | 0.95              |
| 6:O8:20:SER:OG       | 6:O8:22:ASP:OD1     | 1.84                     | 0.95              |
| 10:C16:586:PRO:CD    | 10:C16:650:ARG:NH1  | 2.29                     | 0.95              |
| 10:C16:1548:ILE:HG12 | 24:D8:1407:PHE:HE2  | 1.29                     | 0.95              |
| 11:A40:156:MET:CA    | 11:A40:555:HIS:CD2  | 2.48                     | 0.95              |
| 10:C:1002:LEU:HD12   | 10:C:1019:ARG:NH1   | 1.81                     | 0.95              |
| 11:A16:707:LEU:CD2   | 11:A16:767:ARG:HH22 | 1.79                     | 0.95              |
| 18:B8:484:TYR:CE2    | 18:B8:556:ILE:HD13  | 2.00                     | 0.95              |
| 18:B8:1439:LYS:NZ    | 24:D32:1257:ASN:CB  | 2.28                     | 0.95              |
| 10:C32:848:CYS:HA    | 10:C32:906:ARG:NH2  | 1.81                     | 0.95              |
| 2:M8:730:GLU:HG2     | 8:L16:504:GLN:HE22  | 1.26                     | 0.95              |
| 6:O:54:VAL:HG13      | 6:O:85:TRP:NE1      | 1.81                     | 0.95              |
| 9:K:601:VAL:HG12     | 9:K:604:SER:OG      | 1.66                     | 0.95              |
| 9:K16:894:LYS:HZ2    | 9:K16:1057:GLU:HB3  | 0.88                     | 0.95              |
| 14:W:598:ILE:CG2     | 14:W:626:LEU:HD22   | 1.96                     | 0.95              |
| 10:C:1625:SER:O      | 10:C:1628:SER:OG    | 1.83                     | 0.95              |
| 10:C8:1625:SER:O     | 10:C8:1628:SER:OG   | 1.83                     | 0.95              |
| 11:A16:91:GLU:OE2    | 18:B:1112:LYS:HD2   | 1.64                     | 0.95              |
| 18:B8:928:ARG:NH1    | 18:B8:969:ASP:O     | 1.99                     | 0.95              |
| 20:E:344:PRO:CA      | 24:D:121:GLU:CD     | 2.38                     | 0.95              |
| 22:I16:131:ARG:HG3   | 23:J16:557:ARG:HH21 | 1.25                     | 0.95              |
| 10:C32:593:ARG:NH1   | 10:C32:655:SER:OG   | 1.98                     | 0.95              |
| 5:P8:55:ARG:HH12     | 5:P8:64:ASP:HB2     | 1.27                     | 0.95              |
| 9:K8:1248:LEU:CD1    | 9:K8:1265:ILE:CD1   | 2.44                     | 0.95              |
| 10:C24:1050:HIS:NE2  | 10:C24:1086:LYS:NZ  | 2.12                     | 0.95              |
| 13:V:902:MET:HE1     | 14:W:777:LEU:HD21   | 1.46                     | 0.95              |
| 10:C:848:CYS:HA      | 10:C:906:ARG:NH2    | 1.81                     | 0.95              |
| 18:B:671:MET:HE2     | 18:B:736:ALA:CB     | 1.97                     | 0.95              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:410:GLN:HE21   | 18:B8:538:ARG:HH22   | 1.06                     | 0.95              |
| 19:48:65:LYS:O       | 19:48:66:ALA:C       | 2.04                     | 0.95              |
| 10:C32:1682:VAL:HG21 | 10:C32:1758:LEU:HD23 | 1.47                     | 0.95              |
| 6:O:173:VAL:HG22     | 6:O:189:LEU:HD13     | 1.44                     | 0.95              |
| 5:P8:70:LYS:NZ       | 6:O8:7:THR:OG1       | 1.98                     | 0.95              |
| 5:P16:70:LYS:NZ      | 6:O16:7:THR:OG1      | 1.98                     | 0.95              |
| 5:P16:112:LEU:HD21   | 5:P16:122:TYR:CD2    | 2.02                     | 0.95              |
| 5:P16:499:TYR:CD2    | 6:O16:178:MET:SD     | 2.60                     | 0.95              |
| 9:K8:601:VAL:HG12    | 9:K8:604:SER:OG      | 1.66                     | 0.95              |
| 9:K8:792:LEU:CD2     | 9:K8:864:ILE:HD11    | 1.96                     | 0.95              |
| 10:C16:848:CYS:HA    | 10:C16:906:ARG:NH2   | 1.81                     | 0.95              |
| 10:C16:1625:SER:O    | 10:C16:1628:SER:OG   | 1.83                     | 0.95              |
| 10:C24:848:CYS:HA    | 10:C24:906:ARG:NH2   | 1.81                     | 0.95              |
| 10:C24:1770:LEU:O    | 10:C24:1836:LYS:HE3  | 1.64                     | 0.95              |
| 10:C8:1271:PHE:CE2   | 10:C8:1284:ASP:CB    | 2.47                     | 0.95              |
| 10:C8:1770:LEU:O     | 10:C8:1836:LYS:HE3   | 1.64                     | 0.95              |
| 2:M16:377:ARG:HH12   | 2:M16:477:ASP:HB3    | 1.23                     | 0.95              |
| 5:P8:592:SER:HG      | 5:P8:598:LEU:HD13    | 1.29                     | 0.95              |
| 6:O8:54:VAL:HG13     | 6:O8:85:TRP:NE1      | 1.81                     | 0.95              |
| 10:C16:1687:GLU:OE2  | 10:C16:1806:ARG:NH2  | 1.97                     | 0.95              |
| 11:A40:798:PHE:HE1   | 11:A40:847:ARG:NH1   | 1.63                     | 0.95              |
| 10:C:1682:VAL:HG21   | 10:C:1758:LEU:HD23   | 1.47                     | 0.95              |
| 11:A16:154:ILE:HD12  | 18:B:1842:VAL:HG13   | 1.45                     | 0.95              |
| 18:B8:664:LEU:HD11   | 18:B8:729:LEU:HD21   | 1.46                     | 0.95              |
| 18:B8:671:MET:HE2    | 18:B8:736:ALA:CB     | 1.97                     | 0.95              |
| 20:E8:353:ILE:HD12   | 20:E8:413:PHE:CG     | 2.00                     | 0.95              |
| 20:E8:355:PRO:HA     | 20:E8:454:MET:CE     | 1.96                     | 0.95              |
| 21:H8:312:GLN:HG2    | 21:H8:316:ILE:HD12   | 1.46                     | 0.95              |
| 10:C32:1002:LEU:HD12 | 10:C32:1019:ARG:NH1  | 1.81                     | 0.95              |
| 1:R8:1442:THR:HG21   | 3:N8:13:ILE:CD1      | 1.97                     | 0.95              |
| 5:P:70:LYS:NZ        | 6:O:7:THR:OG1        | 1.98                     | 0.95              |
| 5:P:499:TYR:CD2      | 6:O:178:MET:SD       | 2.60                     | 0.95              |
| 5:P8:499:TYR:CD2     | 6:O8:178:MET:SD      | 2.60                     | 0.95              |
| 8:L8:1096:GLU:OE1    | 9:K8:996:MET:CB      | 2.13                     | 0.95              |
| 9:K:792:LEU:CG       | 9:K:864:ILE:HD11     | 1.96                     | 0.95              |
| 14:W:649:LEU:CD2     | 15:J:575:ILE:HD13    | 1.89                     | 0.95              |
| 11:A32:519:MET:HE2   | 11:A32:569:MET:HE1   | 1.47                     | 0.95              |
| 21:H:312:GLN:HE22    | 22:I:290:ASP:HB3     | 1.32                     | 0.95              |
| 21:H8:291:VAL:CG1    | 23:J8:657:GLU:CG     | 2.45                     | 0.95              |
| 21:H24:312:GLN:HG2   | 21:H24:316:ILE:HD12  | 1.46                     | 0.95              |
| 1:R:1022:TYR:CE1     | 24:D:1441:PRO:HG3    | 2.02                     | 0.95              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:N8:4:GLN:NE2      | 3:N8:44:GLY:O       | 1.99                     | 0.95              |
| 1:R16:1266:THR:HG23 | 5:P16:680:ILE:HG21  | 1.49                     | 0.95              |
| 2:M16:544:LEU:HD21  | 2:M16:586:ALA:HB1   | 1.10                     | 0.95              |
| 7:Q16:143:ARG:NH1   | 7:Q16:190:PRO:O     | 1.99                     | 0.95              |
| 11:A24:798:PHE:HE1  | 11:A24:847:ARG:NH1  | 1.64                     | 0.95              |
| 10:C24:1074:LEU:HG  | 18:B8:256:VAL:O     | 1.65                     | 0.95              |
| 10:C:620:PRO:HB2    | 10:C:636:VAL:HG13   | 1.49                     | 0.95              |
| 10:C8:586:PRO:CD    | 10:C8:650:ARG:NH1   | 2.29                     | 0.95              |
| 18:B:410:GLN:HE21   | 18:B:538:ARG:HH22   | 1.06                     | 0.95              |
| 18:B8:779:LYS:HE2   | 18:B8:847:GLN:NE2   | 1.82                     | 0.95              |
| 20:E:355:PRO:HA     | 20:E:454:MET:CE     | 1.96                     | 0.95              |
| 2:M:254:LEU:HD21    | 2:M:283:ILE:HG12    | 1.47                     | 0.95              |
| 2:M16:544:LEU:CD2   | 2:M16:586:ALA:CB    | 2.29                     | 0.95              |
| 5:P:313:TRP:HZ2     | 5:P:345:MET:CE      | 1.78                     | 0.95              |
| 5:P16:214:LEU:HD23  | 5:P16:236:VAL:HG11  | 1.46                     | 0.95              |
| 10:C:407:LYS:HE3    | 10:C:465:PHE:CE2    | 2.01                     | 0.95              |
| 10:C8:1002:LEU:HD12 | 10:C8:1019:ARG:NH1  | 1.81                     | 0.95              |
| 10:C32:182:ASP:HB2  | 10:C32:183:PRO:HD2  | 1.49                     | 0.95              |
| 2:M:428:SER:HB3     | 8:L:355:SER:OG      | 1.65                     | 0.95              |
| 1:R16:1442:THR:HG21 | 3:N16:13:ILE:CD1    | 1.97                     | 0.95              |
| 6:O:20:SER:OG       | 6:O:22:ASP:OD1      | 1.84                     | 0.95              |
| 11:A24:388:VAL:H    | 11:A24:459:ARG:HH12 | 1.08                     | 0.95              |
| 10:C24:453:LEU:CD2  | 10:C24:459:LEU:CD2  | 2.15                     | 0.95              |
| 11:A40:36:ASN:ND2   | 22:I16:293:LYS:CE   | 2.30                     | 0.95              |
| 11:A40:519:MET:HE2  | 11:A40:569:MET:HE1  | 1.47                     | 0.95              |
| 14:W:598:ILE:HG12   | 14:W:626:LEU:HD23   | 1.49                     | 0.95              |
| 14:W:698:LEU:CD1    | 15:J:617:LEU:HD23   | 1.96                     | 0.95              |
| 18:B:154:LEU:HD21   | 18:B:224:GLU:CD     | 1.91                     | 0.95              |
| 19:4:4:PHE:HE2      | 19:4:378:TYR:CD1    | 1.84                     | 0.95              |
| 20:E:429:PRO:CG     | 24:D:69:VAL:HA      | 1.97                     | 0.95              |
| 5:P8:16:PHE:CE1     | 6:O8:311:LEU:CD1    | 2.49                     | 0.94              |
| 5:P16:16:PHE:CE1    | 6:O16:311:LEU:CD1   | 2.49                     | 0.94              |
| 5:P16:595:SER:C     | 5:P16:597:GLY:N     | 2.24                     | 0.94              |
| 8:L8:1092:LEU:HD13  | 9:K8:999:PHE:HD2    | 1.32                     | 0.94              |
| 9:K:1248:LEU:CD1    | 9:K:1265:ILE:CD1    | 2.45                     | 0.94              |
| 10:C24:620:PRO:HB3  | 10:C24:636:VAL:HG12 | 1.44                     | 0.94              |
| 12:A:707:LEU:CD2    | 12:A:767:ARG:HH22   | 1.79                     | 0.94              |
| 21:H8:312:GLN:HE22  | 22:I8:290:ASP:HB3   | 1.31                     | 0.94              |
| 21:H16:291:VAL:CG1  | 23:J16:657:GLU:CG   | 2.45                     | 0.94              |
| 24:D:405:GLN:OE1    | 24:D16:10:ARG:HG2   | 1.63                     | 0.94              |
| 12:A48:388:VAL:H    | 12:A48:459:ARG:HH12 | 1.08                     | 0.94              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R:1335:ILE:HG13    | 10:C:1170:VAL:HG21   | 1.48                     | 0.94              |
| 2:M:421:LEU:HD11     | 8:L:346:TRP:CD1      | 2.01                     | 0.94              |
| 1:R8:1265:PHE:HD2    | 5:P8:684:ARG:NH1     | 1.65                     | 0.94              |
| 1:R16:1187:ARG:HH22  | 1:R16:1201:LEU:CD1   | 1.80                     | 0.94              |
| 4:T:160:HIS:NE2      | 4:T:160:HIS:ND1      | 2.15                     | 0.94              |
| 5:P:325:PHE:CE2      | 13:V:771:GLN:NE2     | 2.35                     | 0.94              |
| 9:K:1198:LEU:HD11    | 9:K:1267:LEU:HD22    | 1.48                     | 0.94              |
| 9:K8:578:THR:HG21    | 9:K8:616:ARG:HH21    | 1.27                     | 0.94              |
| 10:C16:1663:SER:HA   | 10:C24:1564:ASP:OD2  | 0.77                     | 0.94              |
| 11:A24:468:VAL:CG2   | 24:D16:1100:GLN:CD   | 2.40                     | 0.94              |
| 11:A40:607:ARG:NH2   | 24:D32:914:PHE:CD1   | 2.34                     | 0.94              |
| 11:A40:707:LEU:CD2   | 11:A40:767:ARG:HH22  | 1.79                     | 0.94              |
| 14:W:606:GLN:O       | 14:W:609:THR:OG1     | 1.84                     | 0.94              |
| 10:C:586:PRO:CD      | 10:C:650:ARG:NH1     | 2.29                     | 0.94              |
| 18:B:671:MET:CE      | 18:B:736:ALA:HB3     | 1.97                     | 0.94              |
| 18:B8:1940:ALA:HB1   | 18:B8:1950:ILE:HD11  | 1.46                     | 0.94              |
| 21:H24:291:VAL:CG1   | 23:J24:657:GLU:CG    | 2.45                     | 0.94              |
| 24:D:1099:ARG:CZ     | 24:D:1149:VAL:CG2    | 2.45                     | 0.94              |
| 2:M:254:LEU:CD2      | 2:M:283:ILE:HG12     | 1.97                     | 0.94              |
| 2:M16:672:TYR:CD2    | 2:M16:680:LYS:NZ     | 2.26                     | 0.94              |
| 5:P8:313:TRP:CZ2     | 5:P8:345:MET:CE      | 2.51                     | 0.94              |
| 5:P8:595:SER:C       | 5:P8:597:GLY:N       | 2.24                     | 0.94              |
| 8:L8:1054:HIS:NE2    | 8:L8:1054:HIS:ND1    | 2.15                     | 0.94              |
| 8:L16:851:PRO:CB     | 9:K16:1283:PRO:HB2   | 1.97                     | 0.94              |
| 10:C16:1682:VAL:HG21 | 10:C16:1758:LEU:HD23 | 1.47                     | 0.94              |
| 12:A:302:GLN:NE2     | 12:A:324:ARG:NH1     | 2.14                     | 0.94              |
| 10:C:35:ASN:HA       | 24:D:1148:LEU:CD1    | 1.96                     | 0.94              |
| 11:A16:212:LYS:HE2   | 11:A16:585:MET:CE    | 1.77                     | 0.94              |
| 11:A16:342:VAL:HG13  | 17:F8:77:TYR:CE1     | 2.02                     | 0.94              |
| 11:A32:342:VAL:HG13  | 17:F24:77:TYR:CE1    | 2.02                     | 0.94              |
| 10:C32:586:PRO:CD    | 10:C32:650:ARG:NH1   | 2.29                     | 0.94              |
| 3:N:4:GLN:NE2        | 3:N:44:GLY:HA2       | 1.81                     | 0.94              |
| 1:R8:1466:LYS:HG2    | 6:O8:160:LEU:CD2     | 1.98                     | 0.94              |
| 1:R16:1449:TRP:HZ3   | 2:M16:160:LEU:HD12   | 1.23                     | 0.94              |
| 7:Q:143:ARG:NH1      | 7:Q:190:PRO:O        | 1.99                     | 0.94              |
| 8:L8:1074:ARG:HD3    | 9:K8:1089:LYS:CG     | 1.97                     | 0.94              |
| 9:K:751:LEU:CD2      | 9:K:754:ARG:HH11     | 1.78                     | 0.94              |
| 9:K:1019:ARG:CD      | 9:K:1059:ARG:HD3     | 1.97                     | 0.94              |
| 9:K8:1028:GLN:OE1    | 9:K8:1037:ALA:HA     | 1.67                     | 0.94              |
| 11:A24:519:MET:HE2   | 11:A24:569:MET:HE1   | 1.47                     | 0.94              |
| 10:C:988:GLN:NE2     | 10:C:1064:PHE:CE1    | 2.36                     | 0.94              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A16:676:TYR:HH    | 24:D16:1395:SER:HA  | 1.25                     | 0.94              |
| 18:B8:410:GLN:NE2    | 18:B8:538:ARG:HH22  | 1.62                     | 0.94              |
| 19:48:4:PHE:HE2      | 19:48:378:TYR:CD1   | 1.84                     | 0.94              |
| 21:H24:322:LEU:HD22  | 22:I24:300:LEU:HD21 | 1.49                     | 0.94              |
| 21:H16:231:HIS:CD2   | 23:J16:596:GLN:HE22 | 1.75                     | 0.94              |
| 1:R16:529:HIS:ND1    | 1:R16:529:HIS:NE2   | 2.15                     | 0.94              |
| 3:N16:4:GLN:NE2      | 3:N16:44:GLY:HA2    | 1.81                     | 0.94              |
| 5:P:313:TRP:CZ2      | 5:P:345:MET:CE      | 2.51                     | 0.94              |
| 5:P:322:CYS:CB       | 13:V:767:GLU:OE1    | 2.14                     | 0.94              |
| 5:P:322:CYS:C        | 13:V:767:GLU:OE2    | 2.10                     | 0.94              |
| 9:K8:1048:GLN:OE1    | 9:K8:1128:ARG:HG2   | 1.67                     | 0.94              |
| 14:W:515:CYS:CB      | 14:W:604:PRO:HD3    | 1.90                     | 0.94              |
| 14:W:711:ARG:NH1     | 10:C8:1609:ASP:CB   | 2.24                     | 0.94              |
| 10:C:453:LEU:CD2     | 10:C:459:LEU:CD2    | 2.15                     | 0.94              |
| 10:C8:249:THR:C      | 10:C8:251:GLY:H     | 1.75                     | 0.94              |
| 18:B:154:LEU:CD2     | 18:B:224:GLU:CD     | 2.40                     | 0.94              |
| 18:B:686:LEU:HD13    | 18:B:790:ASP:CG     | 1.93                     | 0.94              |
| 18:B8:154:LEU:CD2    | 18:B8:224:GLU:CD    | 2.41                     | 0.94              |
| 18:B8:671:MET:CE     | 18:B8:736:ALA:HB3   | 1.97                     | 0.94              |
| 21:H16:312:GLN:HE22  | 22:I16:290:ASP:HB3  | 1.31                     | 0.94              |
| 24:D40:839:GLU:OE2   | 24:D40:971:HIS:HB2  | 1.64                     | 0.94              |
| 1:R8:1112:LYS:HD3    | 5:P8:712:PHE:CE1    | 2.02                     | 0.94              |
| 2:M8:844:VAL:HG22    | 4:T8:660:LEU:CG     | 1.97                     | 0.94              |
| 2:M16:627:TYR:CB     | 3:N16:167:LEU:HD12  | 1.98                     | 0.94              |
| 5:P16:16:PHE:HE1     | 6:O16:311:LEU:HD11  | 1.13                     | 0.94              |
| 10:C16:988:GLN:NE2   | 10:C16:1064:PHE:CE1 | 2.36                     | 0.94              |
| 11:A24:707:LEU:CD2   | 11:A24:767:ARG:HH22 | 1.79                     | 0.94              |
| 11:A40:302:GLN:NE2   | 11:A40:324:ARG:NH1  | 2.14                     | 0.94              |
| 13:V:861:PHE:HB3     | 14:W:741:ARG:NH2    | 1.82                     | 0.94              |
| 14:W:715:ASP:HA      | 10:C8:1568:ARG:CZ   | 1.97                     | 0.94              |
| 10:C:565:ARG:CZ      | 10:C:569:PHE:HD2    | 1.80                     | 0.94              |
| 10:C8:182:ASP:HB2    | 10:C8:183:PRO:HD2   | 1.49                     | 0.94              |
| 11:A16:36:ASN:ND2    | 22:I:293:LYS:CE     | 2.30                     | 0.94              |
| 18:B:779:LYS:HE2     | 18:B:847:GLN:NE2    | 1.82                     | 0.94              |
| 22:I16:146:SER:CB    | 23:J16:574:ARG:NH1  | 2.26                     | 0.94              |
| 2:M:844:VAL:HG22     | 4:T:660:LEU:CG      | 1.98                     | 0.94              |
| 1:R16:1434:VAL:HG13  | 2:M16:176:VAL:CG2   | 1.98                     | 0.94              |
| 2:M16:844:VAL:HG22   | 4:T16:660:LEU:CG    | 1.97                     | 0.94              |
| 7:Q8:27:GLN:NE2      | 7:Q8:33:ARG:HG2     | 1.81                     | 0.94              |
| 6:O16:54:VAL:HG13    | 6:O16:85:TRP:NE1    | 1.81                     | 0.94              |
| 10:C24:1708:ARG:HH21 | 21:H24:275:LYS:HE2  | 1.28                     | 0.94              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A40:468:VAL:CG2   | 24:D32:1100:GLN:CD  | 2.40                     | 0.94              |
| 14:W:586:ILE:HD12    | 15:J:569:ALA:CA     | 1.97                     | 0.94              |
| 10:C8:848:CYS:HA     | 10:C8:906:ARG:NH2   | 1.81                     | 0.94              |
| 10:C8:1439:ILE:CD1   | 10:C8:1457:LEU:HD13 | 1.98                     | 0.94              |
| 18:B:779:LYS:HE3     | 18:B:847:GLN:HE22   | 1.31                     | 0.94              |
| 20:E8:261:PRO:CD     | 20:E8:305:GLU:OE1   | 2.15                     | 0.94              |
| 21:H:291:VAL:CG1     | 23:J32:657:GLU:CG   | 2.45                     | 0.94              |
| 21:H24:231:HIS:CD2   | 23:J24:596:GLN:HE22 | 1.76                     | 0.94              |
| 10:C32:249:THR:C     | 10:C32:251:GLY:H    | 1.75                     | 0.94              |
| 10:C32:611:TRP:CZ2   | 10:C32:670:GLU:OE2  | 2.21                     | 0.94              |
| 1:R:529:HIS:ND1      | 1:R:529:HIS:NE2     | 2.15                     | 0.94              |
| 1:R:1328:LYS:HE3     | 10:C:1177:ARG:NE    | 1.83                     | 0.94              |
| 2:M:411:ILE:O        | 8:L:401:LYS:NZ      | 1.99                     | 0.94              |
| 1:R8:1187:ARG:HH22   | 1:R8:1201:LEU:CD1   | 1.80                     | 0.94              |
| 5:P:179:TYR:HE1      | 5:P:437:GLY:CA      | 1.80                     | 0.94              |
| 7:Q8:241:HIS:NE2     | 7:Q8:258:ARG:CZ     | 2.31                     | 0.94              |
| 8:L16:1054:HIS:NE2   | 8:L16:1054:HIS:ND1  | 2.15                     | 0.94              |
| 8:L16:1069:LEU:HD21  | 9:K16:1086:VAL:CG1  | 1.97                     | 0.94              |
| 9:K:959:TRP:CZ2      | 9:K:992:GLN:HB3     | 2.02                     | 0.94              |
| 9:K:1039:ASP:CG      | 9:K:1096:LYS:HZ3    | 1.74                     | 0.94              |
| 10:C16:1002:LEU:HD12 | 10:C16:1019:ARG:NH1 | 1.81                     | 0.94              |
| 11:A24:302:GLN:NE2   | 11:A24:324:ARG:NH1  | 2.14                     | 0.94              |
| 10:C24:611:TRP:CZ2   | 10:C24:670:GLU:OE2  | 2.21                     | 0.94              |
| 13:V:818:THR:HA      | 13:V:824:TRP:HE1    | 1.33                     | 0.94              |
| 11:A16:302:GLN:NE2   | 11:A16:324:ARG:NH1  | 2.14                     | 0.94              |
| 17:F24:74:ILE:C      | 17:F24:76:ASP:H     | 1.75                     | 0.94              |
| 18:B8:154:LEU:HD21   | 18:B8:224:GLU:CD    | 1.91                     | 0.94              |
| 20:E:261:PRO:CD      | 20:E:305:GLU:OE1    | 2.15                     | 0.94              |
| 24:D:308:ASN:HD21    | 24:D16:753:ARG:HE   | 1.11                     | 0.94              |
| 1:R:1187:ARG:HH22    | 1:R:1201:LEU:CD1    | 1.80                     | 0.94              |
| 7:Q:27:GLN:NE2       | 7:Q:33:ARG:HG2      | 1.81                     | 0.94              |
| 5:P16:105:ARG:NH2    | 5:P16:133:TYR:CG    | 2.36                     | 0.94              |
| 9:K:578:THR:HG21     | 9:K:616:ARG:HH21    | 1.27                     | 0.94              |
| 9:K:1028:GLN:OE1     | 9:K:1037:ALA:HA     | 1.67                     | 0.94              |
| 9:K:1232:LEU:HD21    | 9:K:1265:ILE:HG22   | 0.94                     | 0.94              |
| 12:A:212:LYS:HE3     | 12:A:585:MET:HE1    | 1.27                     | 0.94              |
| 13:V:817:GLN:O       | 13:V:820:ASP:N      | 2.00                     | 0.94              |
| 10:C8:620:PRO:HB2    | 10:C8:636:VAL:HG13  | 1.49                     | 0.94              |
| 11:A32:90:PHE:CG     | 18:B8:1788:ILE:HD13 | 2.03                     | 0.94              |
| 10:C32:389:LEU:HD21  | 10:C32:447:PHE:CE1  | 2.03                     | 0.94              |
| 2:M:672:TYR:CB       | 2:M:680:LYS:HD3     | 1.95                     | 0.94              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:540:TYR:HE1   | 2:M16:555:LEU:HD23   | 1.24                     | 0.94              |
| 5:P:152:ILE:HD13    | 14:W:762:GLN:NE2     | 1.83                     | 0.94              |
| 8:L:1054:HIS:ND1    | 8:L:1054:HIS:NE2     | 2.15                     | 0.94              |
| 10:C16:1439:ILE:CD1 | 10:C16:1457:LEU:HD13 | 1.98                     | 0.94              |
| 11:A24:212:LYS:HE3  | 11:A24:585:MET:HE1   | 1.27                     | 0.94              |
| 10:C24:620:PRO:HB2  | 10:C24:636:VAL:HG13  | 1.49                     | 0.94              |
| 10:C24:1251:PHE:CZ  | 10:C24:1319:ARG:CZ   | 2.51                     | 0.94              |
| 10:C8:988:GLN:NE2   | 10:C8:1064:PHE:CE1   | 2.36                     | 0.94              |
| 11:A16:90:PHE:C     | 18:B:1800:ARG:HH22   | 1.74                     | 0.94              |
| 11:A16:798:PHE:HE1  | 11:A16:847:ARG:NH1   | 1.64                     | 0.94              |
| 18:B8:1161:LEU:HD11 | 18:B8:1403:ILE:CD1   | 1.98                     | 0.94              |
| 21:H:322:LEU:HD22   | 22:I:300:LEU:HD21    | 1.50                     | 0.94              |
| 12:A48:707:LEU:CD2  | 12:A48:767:ARG:HH22  | 1.79                     | 0.94              |
| 7:Q:124:PHE:CE1     | 7:Q:125:TYR:OH       | 1.98                     | 0.93              |
| 10:C16:1663:SER:HA  | 10:C24:1564:ASP:CG   | 1.91                     | 0.93              |
| 10:C24:988:GLN:NE2  | 10:C24:1064:PHE:CE1  | 2.35                     | 0.93              |
| 14:W:701:LEU:CD1    | 15:J:624:ALA:HB1     | 1.99                     | 0.93              |
| 11:A32:676:TYR:CE2  | 24:D32:1396:PRO:CD   | 2.51                     | 0.93              |
| 2:M:762:LEU:HB2     | 2:M:813:ASN:HD22     | 1.32                     | 0.93              |
| 1:R8:529:HIS:NE2    | 1:R8:529:HIS:ND1     | 2.15                     | 0.93              |
| 1:R8:1166:ASN:ND2   | 5:P8:672:LEU:HD22    | 1.82                     | 0.93              |
| 2:M8:624:ASP:O      | 3:N8:165:GLY:HA3     | 1.69                     | 0.93              |
| 3:N8:4:GLN:NE2      | 3:N8:44:GLY:HA2      | 1.81                     | 0.93              |
| 8:L:601:HIS:HE1     | 8:L:631:LEU:CD2      | 1.72                     | 0.93              |
| 9:K:581:ASP:CB      | 9:K:625:ARG:HH22     | 1.77                     | 0.93              |
| 9:K:634:LEU:HD22    | 9:K:754:ARG:NH1      | 1.80                     | 0.93              |
| 11:A24:36:ASN:ND2   | 22:I8:293:LYS:CE     | 2.30                     | 0.93              |
| 11:A24:342:VAL:HG13 | 17:F:77:TYR:CE1      | 2.02                     | 0.93              |
| 11:A32:122:LYS:HE3  | 18:B8:1757:GLU:OE2   | 1.68                     | 0.93              |
| 10:C32:417:LEU:HB3  | 10:C32:472:ASN:HD22  | 1.32                     | 0.93              |
| 10:C32:988:GLN:NE2  | 10:C32:1064:PHE:CE1  | 2.36                     | 0.93              |
| 1:R:1434:VAL:HG13   | 2:M:176:VAL:CG2      | 1.98                     | 0.93              |
| 7:Q16:241:HIS:NE2   | 7:Q16:258:ARG:CZ     | 2.31                     | 0.93              |
| 8:L16:976:LEU:CD2   | 9:K16:1004:ARG:NE    | 2.26                     | 0.93              |
| 9:K8:792:LEU:CG     | 9:K8:864:ILE:HD11    | 1.97                     | 0.93              |
| 10:C16:389:LEU:HD21 | 10:C16:447:PHE:CE1   | 2.03                     | 0.93              |
| 10:C16:1251:PHE:CZ  | 10:C16:1319:ARG:CZ   | 2.51                     | 0.93              |
| 14:W:515:CYS:SG     | 14:W:604:PRO:HG3     | 1.89                     | 0.93              |
| 10:C:611:TRP:CZ2    | 10:C:670:GLU:OE2     | 2.21                     | 0.93              |
| 10:C:1050:HIS:NE2   | 10:C:1086:LYS:NZ     | 2.12                     | 0.93              |
| 10:C:1251:PHE:CZ    | 10:C:1319:ARG:CZ     | 2.51                     | 0.93              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 17:F:74:ILE:C       | 17:F:76:ASP:H        | 1.75                     | 0.93              |
| 11:A32:676:TYR:CE2  | 24:D32:1395:SER:CB   | 2.36                     | 0.93              |
| 11:A32:707:LEU:CG   | 11:A32:767:ARG:NH2   | 2.29                     | 0.93              |
| 17:F24:71:GLU:C     | 17:F24:73:GLY:H      | 1.76                     | 0.93              |
| 20:E8:345:LEU:HD21  | 24:D40:123:ALA:HB2   | 1.49                     | 0.93              |
| 21:H:291:VAL:CG1    | 23:J32:657:GLU:HG2   | 1.98                     | 0.93              |
| 21:H24:269:PHE:HD1  | 22:I24:205:ARG:HH12  | 0.96                     | 0.93              |
| 10:C16:611:TRP:CZ2  | 10:C16:670:GLU:OE2   | 2.21                     | 0.93              |
| 10:C8:110:ARG:HH11  | 10:C8:118:LEU:HD11   | 1.00                     | 0.93              |
| 10:C8:667:ILE:CD1   | 10:C8:697:HIS:ND1    | 2.32                     | 0.93              |
| 17:F:71:GLU:C       | 17:F:73:GLY:H        | 1.76                     | 0.93              |
| 11:A32:36:ASN:ND2   | 22:I24:293:LYS:CE    | 2.30                     | 0.93              |
| 11:A32:703:ALA:HA   | 24:D32:1398:ARG:CD   | 1.98                     | 0.93              |
| 18:B:112:GLU:OE2    | 18:B:130:MET:HE1     | 1.68                     | 0.93              |
| 19:4:189:LEU:HD13   | 19:4:203:LEU:CG      | 1.98                     | 0.93              |
| 19:4:250:ILE:HG21   | 20:E:165:ARG:NH2     | 1.80                     | 0.93              |
| 20:E8:235:HIS:CE1   | 20:E8:239:LYS:HE3    | 2.04                     | 0.93              |
| 21:H8:291:VAL:CG1   | 23:J8:657:GLU:HG2    | 1.98                     | 0.93              |
| 21:H24:291:VAL:CG1  | 23:J24:657:GLU:HG2   | 1.98                     | 0.93              |
| 22:I24:146:SER:CB   | 23:J24:574:ARG:NH1   | 2.26                     | 0.93              |
| 10:C32:1251:PHE:HZ  | 10:C32:1319:ARG:NH1  | 1.63                     | 0.93              |
| 2:M16:537:ILE:CG1   | 2:M16:558:MET:HE3    | 1.97                     | 0.93              |
| 6:O8:61:LYS:HZ3     | 6:O8:112:ASP:CG      | 1.77                     | 0.93              |
| 7:Q8:297:VAL:CG1    | 7:Q8:301:ARG:CB      | 2.46                     | 0.93              |
| 9:K8:1232:LEU:HD21  | 9:K8:1265:ILE:HG22   | 0.94                     | 0.93              |
| 10:C24:389:LEU:HD21 | 10:C24:447:PHE:CE1   | 2.03                     | 0.93              |
| 10:C24:417:LEU:HB3  | 10:C24:472:ASN:HD22  | 1.32                     | 0.93              |
| 10:C8:1682:VAL:HG21 | 10:C8:1758:LEU:HD23  | 1.47                     | 0.93              |
| 17:F:74:ILE:HG22    | 17:F:76:ASP:HB2      | 1.50                     | 0.93              |
| 11:A32:302:GLN:NE2  | 11:A32:324:ARG:NH1   | 2.14                     | 0.93              |
| 17:F16:71:GLU:C     | 17:F16:73:GLY:H      | 1.76                     | 0.93              |
| 18:B:609:TYR:CD2    | 18:B:610:VAL:CG2     | 2.50                     | 0.93              |
| 1:R8:1188:TYR:OH    | 24:D40:1459:LEU:HD13 | 1.67                     | 0.93              |
| 5:P:318:THR:CG2     | 13:V:763:LYS:HZ1     | 1.82                     | 0.93              |
| 7:Q:241:HIS:NE2     | 7:Q:258:ARG:CZ       | 2.31                     | 0.93              |
| 7:Q16:124:PHE:CE1   | 7:Q16:125:TYR:OH     | 1.98                     | 0.93              |
| 11:A24:156:MET:CA   | 11:A24:555:HIS:CD2   | 2.51                     | 0.93              |
| 14:W:715:ASP:OD1    | 10:C8:1568:ARG:HD3   | 1.68                     | 0.93              |
| 18:B8:779:LYS:HE3   | 18:B8:847:GLN:HE22   | 1.31                     | 0.93              |
| 18:B8:786:ASP:OD2   | 24:D32:1066:VAL:HA   | 1.68                     | 0.93              |
| 1:R:1442:THR:HG21   | 3:N:13:ILE:CD1       | 1.97                     | 0.93              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P:322:CYS:SG       | 13:V:763:LYS:NZ     | 2.40                     | 0.93              |
| 10:C16:565:ARG:CZ    | 10:C16:569:PHE:HD2  | 1.81                     | 0.93              |
| 10:C16:1002:LEU:HD23 | 10:C16:1012:ARG:CZ  | 1.99                     | 0.93              |
| 11:A24:803:PRO:HB3   | 24:D8:1401:LEU:HD12 | 0.95                     | 0.93              |
| 10:C24:565:ARG:NH1   | 10:C24:568:TRP:HB2  | 1.84                     | 0.93              |
| 10:C:182:ASP:HB2     | 10:C:183:PRO:HD2    | 1.49                     | 0.93              |
| 10:C8:611:TRP:CZ2    | 10:C8:670:GLU:OE2   | 2.21                     | 0.93              |
| 20:E:344:PRO:CA      | 24:D:121:GLU:OE2    | 2.13                     | 0.93              |
| 19:48:189:LEU:HD13   | 19:48:203:LEU:CG    | 1.98                     | 0.93              |
| 1:R:1132:TYR:CZ      | 1:R:1214:ILE:HD13   | 2.04                     | 0.93              |
| 1:R8:1434:VAL:HG13   | 2:M8:176:VAL:CG2    | 1.98                     | 0.93              |
| 10:C16:390:HIS:CD2   | 10:C16:452:LEU:HD13 | 2.02                     | 0.93              |
| 14:W:645:HIS:CE1     | 14:W:649:LEU:HD12   | 2.02                     | 0.93              |
| 10:C:1265:ARG:O      | 10:C:1268:ARG:NE    | 2.02                     | 0.93              |
| 17:F8:71:GLU:C       | 17:F8:73:GLY:H      | 1.76                     | 0.93              |
| 18:B8:112:GLU:OE2    | 18:B8:130:MET:HE1   | 1.68                     | 0.93              |
| 21:H8:193:LEU:HD21   | 21:H8:195:GLN:HE21  | 1.34                     | 0.93              |
| 24:D:44:SER:HB3      | 24:D16:761:ASN:HD22 | 1.34                     | 0.93              |
| 10:C32:389:LEU:CD2   | 10:C32:447:PHE:HE1  | 1.82                     | 0.93              |
| 1:R:1269:LEU:HD12    | 5:P:684:ARG:NE      | 1.84                     | 0.93              |
| 2:M:624:ASP:O        | 3:N:165:GLY:HA3     | 1.69                     | 0.93              |
| 2:M16:408:GLU:OE1    | 8:L16:484:PRO:HG3   | 1.69                     | 0.93              |
| 9:K:649:MET:HB3      | 9:K:704:ARG:HH21    | 1.01                     | 0.93              |
| 10:C16:417:LEU:HB3   | 10:C16:472:ASN:HD22 | 1.32                     | 0.93              |
| 10:C8:960:PHE:HZ     | 10:C8:1138:GLU:CD   | 1.68                     | 0.93              |
| 18:B8:32:LEU:CD1     | 18:B8:163:ILE:HD12  | 1.99                     | 0.93              |
| 20:E:235:HIS:CE1     | 20:E:239:LYS:HE3    | 2.04                     | 0.93              |
| 22:I:146:SER:CB      | 23:J32:574:ARG:NH1  | 2.26                     | 0.93              |
| 23:J8:623:GLU:OE1    | 23:J8:626:ARG:NH2   | 2.02                     | 0.93              |
| 10:C32:1002:LEU:HD23 | 10:C32:1012:ARG:CZ  | 1.99                     | 0.93              |
| 2:M16:816:ARG:NH1    | 2:M16:849:LEU:CB    | 2.24                     | 0.93              |
| 5:P8:614:VAL:CG2     | 5:P8:629:ARG:CZ     | 2.47                     | 0.93              |
| 10:C24:249:THR:C     | 10:C24:251:GLY:H    | 1.75                     | 0.93              |
| 11:A40:388:VAL:H     | 11:A40:459:ARG:HH12 | 1.08                     | 0.93              |
| 10:C8:1002:LEU:HD23  | 10:C8:1012:ARG:CZ   | 1.99                     | 0.93              |
| 11:A16:122:LYS:HE3   | 18:B:1757:GLU:OE2   | 1.68                     | 0.93              |
| 18:B8:686:LEU:HD13   | 18:B8:790:ASP:CG    | 1.93                     | 0.93              |
| 22:I:131:ARG:HG3     | 23:J32:557:ARG:HH21 | 1.25                     | 0.93              |
| 21:H16:291:VAL:CG1   | 23:J16:657:GLU:HG2  | 1.98                     | 0.93              |
| 10:C32:1050:HIS:CD2  | 10:C32:1086:LYS:HZ1 | 1.84                     | 0.93              |
| 1:R8:1132:TYR:CZ     | 1:R8:1214:ILE:HD13  | 2.04                     | 0.92              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 1:R8:1188:TYR:CZ     | 24:D40:1459:LEU:CB  | 2.51                     | 0.92              |
| 1:R16:1132:TYR:CZ    | 1:R16:1214:ILE:HD13 | 2.03                     | 0.92              |
| 9:K8:1198:LEU:HD11   | 9:K8:1267:LEU:HD22  | 1.48                     | 0.92              |
| 13:V:902:MET:CE      | 14:W:777:LEU:HD21   | 1.97                     | 0.92              |
| 10:C:561:ASN:OD1     | 10:C:562:PRO:HD2    | 1.69                     | 0.92              |
| 19:48:189:LEU:CG     | 19:48:203:LEU:HD23  | 1.99                     | 0.92              |
| 24:D:387:LEU:HB2     | 24:D16:746:ALA:CB   | 1.99                     | 0.92              |
| 10:C32:1251:PHE:CZ   | 10:C32:1319:ARG:CZ  | 2.52                     | 0.92              |
| 4:T8:160:HIS:ND1     | 4:T8:160:HIS:NE2    | 2.15                     | 0.92              |
| 4:T16:160:HIS:NE2    | 4:T16:160:HIS:ND1   | 2.16                     | 0.92              |
| 10:C16:1265:ARG:O    | 10:C16:1268:ARG:NE  | 2.02                     | 0.92              |
| 11:A24:603:ALA:O     | 11:A24:616:ARG:NH1  | 2.03                     | 0.92              |
| 10:C8:225:LEU:CD2    | 10:C8:388:TYR:OH    | 2.18                     | 0.92              |
| 11:A16:36:ASN:HD21   | 22:I:293:LYS:CE     | 1.83                     | 0.92              |
| 11:A16:707:LEU:CB    | 24:D16:1398:ARG:NH2 | 2.32                     | 0.92              |
| 17:F8:74:ILE:HG22    | 17:F8:76:ASP:HB2    | 1.51                     | 0.92              |
| 18:B8:729:LEU:HD13   | 18:B8:1196:MET:CE   | 1.99                     | 0.92              |
| 19:4:189:LEU:CG      | 19:4:203:LEU:HD23   | 1.99                     | 0.92              |
| 21:H8:322:LEU:HD22   | 22:I8:300:LEU:HD21  | 1.49                     | 0.92              |
| 23:J16:623:GLU:OE1   | 23:J16:626:ARG:NH2  | 2.02                     | 0.92              |
| 12:A48:629:LEU:C     | 12:A48:678:LYS:NZ   | 2.27                     | 0.92              |
| 3:N:162:THR:CG2      | 3:N:168:VAL:HG22    | 1.83                     | 0.92              |
| 2:M16:340:GLU:OE1    | 4:T8:635:ALA:CB     | 2.17                     | 0.92              |
| 2:M16:624:ASP:O      | 3:N16:165:GLY:HA3   | 1.69                     | 0.92              |
| 4:T:672:GLN:CG       | 5:P:702:LEU:HD21    | 1.99                     | 0.92              |
| 7:Q16:297:VAL:CG1    | 7:Q16:301:ARG:CB    | 2.46                     | 0.92              |
| 8:L16:1071:LEU:CD2   | 9:K16:1284:MET:SD   | 2.58                     | 0.92              |
| 9:K8:1117:LEU:HG     | 9:K8:1139:ILE:HD11  | 1.51                     | 0.92              |
| 10:C24:1002:LEU:HD23 | 10:C24:1012:ARG:CZ  | 1.99                     | 0.92              |
| 14:W:627:PHE:HZ      | 15:J:554:LEU:HD13   | 1.28                     | 0.92              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:CD1   | 1.98                     | 0.92              |
| 18:B:1161:LEU:HD12   | 18:B:1403:ILE:HG21  | 1.46                     | 0.92              |
| 18:B:1528:PRO:HA     | 18:B:1531:TRP:NE1   | 1.85                     | 0.92              |
| 18:B8:1529:GLU:OE2   | 24:D32:1415:LEU:HG  | 1.68                     | 0.92              |
| 21:H16:193:LEU:HD21  | 21:H16:195:GLN:HE21 | 1.34                     | 0.92              |
| 24:D8:1330:ARG:NH1   | 24:D16:719:ARG:CB   | 2.32                     | 0.92              |
| 10:C32:561:ASN:OD1   | 10:C32:562:PRO:HD2  | 1.69                     | 0.92              |
| 2:M:844:VAL:HG22     | 4:T:660:LEU:CD1     | 1.99                     | 0.92              |
| 2:M16:544:LEU:HD21   | 2:M16:586:ALA:HB3   | 1.45                     | 0.92              |
| 5:P8:247:GLU:OE2     | 5:P8:247:GLU:N      | 2.02                     | 0.92              |
| 5:P16:313:TRP:CZ2    | 5:P16:345:MET:CE    | 2.51                     | 0.92              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 8:L:346:TRP:CH2      | 8:L:350:THR:HG21     | 2.04                     | 0.92              |
| 8:L16:1096:GLU:CD    | 9:K16:998:GLN:CG     | 2.43                     | 0.92              |
| 10:C24:1133:ILE:HG13 | 10:C24:1152:LYS:HZ2  | 1.33                     | 0.92              |
| 11:A40:342:VAL:HG13  | 17:F16:77:TYR:CE1    | 2.02                     | 0.92              |
| 10:C:1133:ILE:HG13   | 10:C:1152:LYS:HZ2    | 1.33                     | 0.92              |
| 10:C8:1251:PHE:CZ    | 10:C8:1319:ARG:CZ    | 2.51                     | 0.92              |
| 11:A16:707:LEU:HB2   | 24:D16:1398:ARG:HH22 | 1.27                     | 0.92              |
| 11:A32:36:ASN:HD21   | 22:I24:293:LYS:CE    | 1.83                     | 0.92              |
| 17:F16:74:ILE:C      | 17:F16:76:ASP:H      | 1.75                     | 0.92              |
| 18:B:846:SER:HG      | 18:B:899:LYS:HZ3     | 1.03                     | 0.92              |
| 18:B8:686:LEU:CD1    | 18:B8:790:ASP:CG     | 2.43                     | 0.92              |
| 18:B8:1161:LEU:HD12  | 18:B8:1403:ILE:HG21  | 1.46                     | 0.92              |
| 2:M16:428:SER:HB3    | 8:L16:355:SER:OG     | 1.68                     | 0.92              |
| 2:M16:625:HIS:NE2    | 3:N16:225:PRO:HA     | 1.85                     | 0.92              |
| 5:P:401:ARG:NH2      | 5:P:404:ILE:HG21     | 1.85                     | 0.92              |
| 7:Q:297:VAL:CG1      | 7:Q:301:ARG:CB       | 2.46                     | 0.92              |
| 9:K8:792:LEU:HD23    | 9:K8:864:ILE:HD11    | 1.51                     | 0.92              |
| 10:C16:225:LEU:CD2   | 10:C16:388:TYR:OH    | 2.17                     | 0.92              |
| 10:C16:389:LEU:CD2   | 10:C16:447:PHE:HE1   | 1.82                     | 0.92              |
| 10:C24:1814:LYS:HZ3  | 23:J24:738:MET:CB    | 1.77                     | 0.92              |
| 14:W:701:LEU:HD11    | 15:J:624:ALA:CB      | 1.99                     | 0.92              |
| 10:C:225:LEU:CD2     | 10:C:388:TYR:OH      | 2.18                     | 0.92              |
| 10:C:966:CYS:SG      | 10:C:1021:TRP:CE3    | 2.63                     | 0.92              |
| 10:C:966:CYS:SG      | 10:C:1021:TRP:HE3    | 1.92                     | 0.92              |
| 18:B:686:LEU:CD1     | 18:B:790:ASP:CG      | 2.43                     | 0.92              |
| 18:B:729:LEU:HD13    | 18:B:1196:MET:CE     | 1.99                     | 0.92              |
| 23:J32:623:GLU:OE1   | 23:J32:626:ARG:NH2   | 2.02                     | 0.92              |
| 10:C32:1265:ARG:O    | 10:C32:1268:ARG:NE   | 2.02                     | 0.92              |
| 1:R:1075:LYS:HE2     | 5:P:713:LEU:O        | 0.74                     | 0.92              |
| 2:M:385:LEU:HD11     | 2:M:396:PHE:CD2      | 2.04                     | 0.92              |
| 2:M8:385:LEU:HD11    | 2:M8:396:PHE:CD2     | 2.04                     | 0.92              |
| 7:Q:221:TRP:CZ3      | 7:Q:222:PHE:CE2      | 2.58                     | 0.92              |
| 5:P16:610:SER:HB3    | 5:P16:625:GLU:OE1    | 1.70                     | 0.92              |
| 7:Q16:187:TRP:CH2    | 7:Q16:207:GLN:NE2    | 2.38                     | 0.92              |
| 10:C16:565:ARG:NH1   | 10:C16:568:TRP:HB2   | 1.84                     | 0.92              |
| 10:C16:620:PRO:HB2   | 10:C16:636:VAL:HG13  | 1.49                     | 0.92              |
| 10:C24:345:MET:HE2   | 10:C24:401:ILE:HD11  | 1.51                     | 0.92              |
| 11:A40:36:ASN:HD21   | 22:I16:293:LYS:CE    | 1.83                     | 0.92              |
| 10:C32:1439:ILE:CD1  | 10:C32:1457:LEU:HD13 | 1.98                     | 0.92              |
| 1:R8:1166:ASN:HD21   | 5:P8:672:LEU:HD22    | 1.35                     | 0.92              |
| 5:P:595:SER:C        | 5:P:597:GLY:N        | 2.24                     | 0.92              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P8:614:VAL:HB      | 5:P8:629:ARG:NE      | 1.83                     | 0.92              |
| 8:L16:1071:LEU:HD21  | 9:K16:1284:MET:CE    | 1.99                     | 0.92              |
| 9:K:1048:GLN:OE1     | 9:K:1128:ARG:HG2     | 1.67                     | 0.92              |
| 10:C16:667:ILE:HD13  | 10:C16:697:HIS:CE1   | 1.94                     | 0.92              |
| 10:C24:225:LEU:CD2   | 10:C24:388:TYR:OH    | 2.18                     | 0.92              |
| 11:A40:326:TYR:HD1   | 17:F16:77:TYR:CB     | 1.83                     | 0.92              |
| 10:C:1439:ILE:CD1    | 10:C:1457:LEU:HD13   | 1.98                     | 0.92              |
| 11:A16:711:ARG:CZ    | 24:D16:1399:SER:H    | 1.71                     | 0.92              |
| 11:A32:112:ALA:HB1   | 18:B8:1416:LYS:NZ    | 1.83                     | 0.92              |
| 17:F24:74:ILE:HG22   | 17:F24:76:ASP:HB2    | 1.50                     | 0.92              |
| 19:48:153:ARG:NH2    | 20:E8:467:ILE:CD1    | 2.32                     | 0.92              |
| 10:C32:225:LEU:CD2   | 10:C32:388:TYR:OH    | 2.17                     | 0.92              |
| 10:C32:620:PRO:HB2   | 10:C32:636:VAL:HG13  | 1.49                     | 0.92              |
| 2:M8:534:HIS:CD2     | 2:M8:557:THR:CG2     | 2.52                     | 0.92              |
| 7:Q8:187:TRP:CH2     | 7:Q8:207:GLN:NE2     | 2.38                     | 0.92              |
| 8:L16:976:LEU:HD22   | 9:K16:1004:ARG:CD    | 1.92                     | 0.92              |
| 10:C24:182:ASP:HB2   | 10:C24:183:PRO:HD2   | 1.49                     | 0.92              |
| 10:C24:561:ASN:OD1   | 10:C24:562:PRO:HD2   | 1.69                     | 0.92              |
| 10:C24:1439:ILE:CD1  | 10:C24:1457:LEU:HD13 | 1.98                     | 0.92              |
| 11:A40:629:LEU:C     | 11:A40:678:LYS:NZ    | 2.27                     | 0.92              |
| 11:A16:603:ALA:O     | 11:A16:616:ARG:NH1   | 2.03                     | 0.92              |
| 11:A16:629:LEU:C     | 11:A16:678:LYS:NZ    | 2.27                     | 0.92              |
| 18:B8:313:ILE:HD12   | 18:B8:331:TRP:CD2    | 2.05                     | 0.92              |
| 10:C32:345:MET:HE2   | 10:C32:401:ILE:HD11  | 1.52                     | 0.92              |
| 1:R:1369:LEU:CD1     | 6:O:211:ASN:CG       | 2.40                     | 0.92              |
| 2:M8:625:HIS:NE2     | 3:N8:225:PRO:HA      | 1.84                     | 0.92              |
| 10:C16:453:LEU:CD2   | 10:C16:459:LEU:CD2   | 2.15                     | 0.92              |
| 11:A24:36:ASN:HD21   | 22:I8:293:LYS:CE     | 1.83                     | 0.92              |
| 13:V:844:MET:HG3     | 10:C8:1502:ARG:NH2   | 1.84                     | 0.92              |
| 14:W:645:HIS:HE1     | 14:W:649:LEU:HD11    | 1.33                     | 0.92              |
| 10:C8:1121:ILE:HG22  | 10:C8:1133:ILE:HD13  | 1.52                     | 0.92              |
| 11:A32:714:GLY:HA3   | 24:D32:1398:ARG:HH21 | 1.34                     | 0.92              |
| 18:B:32:LEU:CD1      | 18:B:163:ILE:HD12    | 1.99                     | 0.92              |
| 18:B:514:THR:CG2     | 18:B:549:TRP:CH2     | 2.53                     | 0.92              |
| 24:D:409:LEU:CD1     | 24:D16:746:ALA:H     | 1.81                     | 0.92              |
| 10:C32:1285:VAL:HG23 | 10:C32:1738:MET:HE1  | 1.52                     | 0.92              |
| 10:C32:1466:ARG:HA   | 10:C32:1469:HIS:HE1  | 1.31                     | 0.92              |
| 2:M8:377:ARG:HH12    | 2:M8:477:ASP:HB3     | 1.23                     | 0.92              |
| 3:N16:19:MET:HE2     | 3:N16:23:GLY:O       | 1.70                     | 0.92              |
| 7:Q:187:TRP:CH2      | 7:Q:207:GLN:NE2      | 2.38                     | 0.92              |
| 6:O16:54:VAL:HG13    | 6:O16:85:TRP:HE1     | 1.33                     | 0.92              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A24:390:ALA:HB1   | 24:D16:1099:ARG:HB2  | 1.52                     | 0.92              |
| 10:C:1010:ALA:CA     | 10:C:1192:ARG:NH2    | 2.33                     | 0.92              |
| 10:C:1121:ILE:HG22   | 10:C:1133:ILE:HD13   | 1.52                     | 0.92              |
| 10:C8:1265:ARG:O     | 10:C8:1268:ARG:NE    | 2.02                     | 0.92              |
| 10:C8:1757:GLN:OE1   | 16:A8:136:LEU:CD2    | 2.18                     | 0.92              |
| 11:A16:91:GLU:CB     | 18:B:1112:LYS:CE     | 2.34                     | 0.92              |
| 11:A16:112:ALA:HB1   | 18:B:1416:LYS:NZ     | 1.83                     | 0.92              |
| 11:A32:603:ALA:O     | 11:A32:616:ARG:NH1   | 2.03                     | 0.92              |
| 11:A32:629:LEU:C     | 11:A32:678:LYS:NZ    | 2.27                     | 0.92              |
| 18:B:1210:CYS:HG     | 18:B:1234:MET:HE1    | 1.28                     | 0.92              |
| 18:B8:1528:PRO:HA    | 18:B8:1531:TRP:NE1   | 1.85                     | 0.92              |
| 23:J24:623:GLU:OE1   | 23:J24:626:ARG:NH2   | 2.02                     | 0.92              |
| 1:R:1324:ASP:OD2     | 10:C:1180:ILE:HG22   | 1.67                     | 0.91              |
| 2:M8:627:TYR:CB      | 3:N8:167:LEU:HD12    | 1.99                     | 0.91              |
| 5:P8:15:LEU:HD23     | 6:O8:309:SER:O       | 1.69                     | 0.91              |
| 5:P16:15:LEU:HD23    | 6:O16:309:SER:O      | 1.69                     | 0.91              |
| 9:K:1160:ARG:NH2     | 9:K:1220:ASN:ND2     | 2.18                     | 0.91              |
| 10:C16:182:ASP:HB2   | 10:C16:183:PRO:HD2   | 1.49                     | 0.91              |
| 10:C16:249:THR:C     | 10:C16:251:GLY:H     | 1.75                     | 0.91              |
| 10:C16:1251:PHE:HZ   | 10:C16:1319:ARG:NH1  | 1.63                     | 0.91              |
| 10:C24:565:ARG:CZ    | 10:C24:569:PHE:HD2   | 1.81                     | 0.91              |
| 10:C24:1265:ARG:O    | 10:C24:1268:ARG:NE   | 2.02                     | 0.91              |
| 10:C8:1466:ARG:HA    | 10:C8:1469:HIS:HE1   | 1.32                     | 0.91              |
| 18:B:1419:LYS:HG3    | 18:B:1468:PHE:HE1    | 1.33                     | 0.91              |
| 19:4:153:ARG:NH2     | 20:E:467:ILE:CD1     | 2.32                     | 0.91              |
| 24:D24:1452:LYS:HZ1  | 24:D32:971:HIS:CE1   | 1.87                     | 0.91              |
| 6:O:119:ARG:HH21     | 6:O:182:GLU:HG2      | 1.25                     | 0.91              |
| 8:L8:601:HIS:CE1     | 8:L8:631:LEU:HB2     | 2.05                     | 0.91              |
| 10:C16:1010:ALA:CA   | 10:C16:1192:ARG:NH2  | 2.33                     | 0.91              |
| 10:C16:1163:LEU:HD23 | 10:C16:1166:SER:CB   | 2.00                     | 0.91              |
| 10:C24:1757:GLN:OE1  | 11:A40:136:LEU:CD2   | 2.19                     | 0.91              |
| 18:B:313:ILE:HD12    | 18:B:331:TRP:CD2     | 2.05                     | 0.91              |
| 18:B:643:MET:CE      | 18:B:711:CYS:HB3     | 2.00                     | 0.91              |
| 18:B:1028:LYS:NZ     | 18:B:1092:GLU:OE2    | 2.03                     | 0.91              |
| 1:R:1139:ARG:HD3     | 1:R:1157:ARG:NH2     | 1.83                     | 0.91              |
| 1:R8:1059:ILE:HG21   | 24:D40:1435:ARG:HH21 | 1.31                     | 0.91              |
| 6:O:54:VAL:HG13      | 6:O:85:TRP:HE1       | 1.32                     | 0.91              |
| 6:O16:119:ARG:HH21   | 6:O16:182:GLU:HG2    | 1.25                     | 0.91              |
| 8:L16:851:PRO:CG     | 9:K16:1283:PRO:HB2   | 2.00                     | 0.91              |
| 11:A40:36:ASN:HD22   | 22:I16:293:LYS:NZ    | 1.68                     | 0.91              |
| 11:A40:468:VAL:CG2   | 24:D32:1100:GLN:OE1  | 2.18                     | 0.91              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A40:603:ALA:O     | 11:A40:616:ARG:NH1   | 2.03                     | 0.91              |
| 10:C8:228:ARG:NH2    | 10:C8:277:SER:HB3    | 1.85                     | 0.91              |
| 22:I24:289:LEU:HD23  | 22:I24:296:ARG:HH22  | 1.34                     | 0.91              |
| 10:C32:1163:LEU:HD23 | 10:C32:1166:SER:CB   | 2.00                     | 0.91              |
| 1:R:1185:THR:CG2     | 24:D:1462:PHE:HZ     | 1.82                     | 0.91              |
| 1:R:1326:GLY:HA3     | 10:C:1154:TRP:CE2    | 2.04                     | 0.91              |
| 5:P:109:ILE:HG12     | 14:W:18:PRO:HG3      | 0.91                     | 0.91              |
| 6:O16:61:LYS:HZ3     | 6:O16:112:ASP:CG     | 1.76                     | 0.91              |
| 8:L16:1096:GLU:OE1   | 9:K16:998:GLN:CG     | 2.19                     | 0.91              |
| 10:C24:394:SER:OG    | 10:C24:452:LEU:HD11  | 1.70                     | 0.91              |
| 10:C:565:ARG:NH1     | 10:C:568:TRP:HB2     | 1.84                     | 0.91              |
| 18:B:171:ILE:HD13    | 18:B:226:TYR:HB3     | 1.53                     | 0.91              |
| 18:B:750:GLU:OE1     | 18:B:760:ARG:NH2     | 2.04                     | 0.91              |
| 24:D40:839:GLU:HB3   | 24:D40:971:HIS:CD2   | 2.03                     | 0.91              |
| 10:C32:653:TYR:OH    | 10:C32:679:ARG:HB3   | 1.70                     | 0.91              |
| 2:M:627:TYR:CB       | 3:N:167:LEU:HD12     | 1.99                     | 0.91              |
| 3:N:1:MET:CB         | 3:N:302:PRO:C        | 2.43                     | 0.91              |
| 2:M8:847:PHE:CB      | 4:T8:656:TRP:CE3     | 2.32                     | 0.91              |
| 10:C16:1814:LYS:HE2  | 23:J32:738:MET:CE    | 2.01                     | 0.91              |
| 10:C24:1010:ALA:CA   | 10:C24:1192:ARG:NH2  | 2.33                     | 0.91              |
| 11:A40:707:LEU:CG    | 11:A40:767:ARG:NH2   | 2.29                     | 0.91              |
| 10:C:1002:LEU:HD23   | 10:C:1012:ARG:CZ     | 1.99                     | 0.91              |
| 10:C8:807:GLN:OE1    | 10:C8:811:ILE:HG21   | 1.71                     | 0.91              |
| 11:A16:36:ASN:HD22   | 22:I:293:LYS:NZ      | 1.68                     | 0.91              |
| 18:B:112:GLU:OE1     | 18:B:130:MET:SD      | 2.29                     | 0.91              |
| 18:B:968:PHE:HB2     | 18:B:1040:MET:CE     | 1.99                     | 0.91              |
| 18:B8:112:GLU:OE1    | 18:B8:130:MET:SD     | 2.29                     | 0.91              |
| 22:I:210:LYS:C       | 22:I8:139:GLN:NE2    | 2.28                     | 0.91              |
| 21:H16:322:LEU:HD22  | 22:I16:300:LEU:HD21  | 1.49                     | 0.91              |
| 22:I16:289:LEU:HD23  | 22:I16:296:ARG:HH22  | 1.34                     | 0.91              |
| 1:R:1033:LYS:CE      | 24:D:1432:THR:HB     | 2.00                     | 0.91              |
| 1:R8:1139:ARG:NH2    | 1:R8:1226:THR:OG1    | 2.02                     | 0.91              |
| 3:N16:270:THR:OG1    | 3:N16:272:ASN:OD1    | 1.89                     | 0.91              |
| 5:P:318:THR:CG2      | 13:V:763:LYS:NZ      | 2.33                     | 0.91              |
| 6:O:61:LYS:HZ3       | 6:O:112:ASP:CG       | 1.79                     | 0.91              |
| 5:P8:16:PHE:CD1      | 6:O8:311:LEU:CD1     | 2.54                     | 0.91              |
| 11:A24:707:LEU:CG    | 11:A24:767:ARG:NH2   | 2.29                     | 0.91              |
| 11:A40:748:GLU:HB3   | 24:D24:1398:ARG:HH12 | 0.77                     | 0.91              |
| 17:F8:74:ILE:C       | 17:F8:76:ASP:H       | 1.75                     | 0.91              |
| 18:B8:968:PHE:HB2    | 18:B8:1040:MET:CE    | 1.99                     | 0.91              |
| 23:J8:686:MET:HE1    | 23:J8:694:ARG:NE     | 1.86                     | 0.91              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M:627:TYR:HB3      | 3:N:167:LEU:CD1     | 2.01                     | 0.91              |
| 1:R16:1460:MET:HE2   | 1:R16:1463:GLN:OE1  | 1.71                     | 0.91              |
| 2:M16:627:TYR:HB3    | 3:N16:167:LEU:CD1   | 2.00                     | 0.91              |
| 5:P:633:LEU:HD21     | 5:P:639:THR:HG21    | 1.52                     | 0.91              |
| 5:P8:105:ARG:CZ      | 5:P8:130:VAL:HA     | 2.00                     | 0.91              |
| 10:C16:1548:ILE:HD12 | 24:D8:1407:PHE:HZ   | 1.35                     | 0.91              |
| 10:C16:1757:GLN:OE1  | 11:A24:136:LEU:CD2  | 2.19                     | 0.91              |
| 11:A24:36:ASN:HD22   | 22:I8:293:LYS:NZ    | 1.68                     | 0.91              |
| 12:A:388:VAL:H       | 12:A:459:ARG:HH12   | 1.08                     | 0.91              |
| 12:A:603:ALA:O       | 12:A:616:ARG:NH1    | 2.03                     | 0.91              |
| 19:48:250:ILE:CG1    | 20:E8:165:ARG:NH2   | 2.34                     | 0.91              |
| 21:H:269:PHE:HD1     | 22:I:205:ARG:HH12   | 0.96                     | 0.91              |
| 1:R:1290:ILE:CD1     | 10:C:605:GLU:CD     | 2.42                     | 0.91              |
| 5:P:251:LYS:HZ1      | 14:W:765:LYS:NZ     | 1.68                     | 0.91              |
| 7:Q8:221:TRP:CZ3     | 7:Q8:222:PHE:CE2    | 2.58                     | 0.91              |
| 5:P16:247:GLU:N      | 5:P16:247:GLU:OE2   | 2.02                     | 0.91              |
| 10:C16:807:GLN:OE1   | 10:C16:811:ILE:HG21 | 1.71                     | 0.91              |
| 10:C16:1688:ARG:CG   | 23:J32:735:LYS:CE   | 2.44                     | 0.91              |
| 10:C24:389:LEU:CD2   | 10:C24:447:PHE:HE1  | 1.82                     | 0.91              |
| 10:C24:1163:LEU:HD23 | 10:C24:1166:SER:CB  | 2.00                     | 0.91              |
| 10:C24:1251:PHE:HZ   | 10:C24:1319:ARG:NH1 | 1.62                     | 0.91              |
| 10:C8:561:ASN:OD1    | 10:C8:562:PRO:HD2   | 1.69                     | 0.91              |
| 10:C8:1010:ALA:CA    | 10:C8:1192:ARG:NH2  | 2.33                     | 0.91              |
| 10:C8:1163:LEU:HD23  | 10:C8:1166:SER:CB   | 2.00                     | 0.91              |
| 10:C8:1271:PHE:HZ    | 10:C8:1284:ASP:CG   | 1.74                     | 0.91              |
| 11:A16:711:ARG:CZ    | 24:D16:1399:SER:N   | 2.29                     | 0.91              |
| 11:A32:326:TYR:HD1   | 17:F24:77:TYR:HB3   | 1.35                     | 0.91              |
| 18:B8:171:ILE:HD13   | 18:B8:226:TYR:HB3   | 1.53                     | 0.91              |
| 24:D40:839:GLU:HB3   | 24:D40:971:HIS:CG   | 2.06                     | 0.91              |
| 10:C32:1133:ILE:HG13 | 10:C32:1152:LYS:HZ2 | 1.36                     | 0.91              |
| 2:M:416:VAL:HG11     | 8:L:398:ALA:CB      | 1.99                     | 0.91              |
| 2:M16:417:ARG:CB     | 8:L16:298:PHE:CE2   | 2.39                     | 0.91              |
| 5:P:247:GLU:N        | 5:P:247:GLU:OE2     | 2.02                     | 0.91              |
| 5:P:600:PHE:CZ       | 5:P:638:SER:HB2     | 2.06                     | 0.91              |
| 9:K:635:ALA:HB2      | 9:K:655:GLN:CD      | 1.96                     | 0.91              |
| 10:C16:561:ASN:OD1   | 10:C16:562:PRO:HD2  | 1.69                     | 0.91              |
| 11:A24:326:TYR:HD1   | 17:F:77:TYR:CB      | 1.83                     | 0.91              |
| 10:C24:653:TYR:OH    | 10:C24:679:ARG:HB3  | 1.70                     | 0.91              |
| 10:C8:643:LEU:HB3    | 10:C8:679:ARG:NH2   | 1.86                     | 0.91              |
| 18:B8:514:THR:CG2    | 18:B8:549:TRP:CH2   | 2.53                     | 0.91              |
| 18:B8:609:TYR:CD2    | 18:B8:610:VAL:CG2   | 2.50                     | 0.91              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B8:1256:THR:CG2  | 24:D32:1238:GLU:CG  | 2.44                     | 0.91              |
| 18:B8:1273:GLU:HG2  | 18:B8:1276:LYS:HE3  | 0.93                     | 0.91              |
| 22:I8:289:LEU:HD23  | 22:I8:296:ARG:HH22  | 1.34                     | 0.91              |
| 1:R:1191:LYS:CD     | 24:D:1453:GLU:OE1   | 2.19                     | 0.91              |
| 2:M8:762:LEU:HB2    | 2:M8:813:ASN:HD22   | 1.32                     | 0.91              |
| 2:M16:385:LEU:HD11  | 2:M16:396:PHE:CD2   | 2.04                     | 0.91              |
| 2:M16:408:GLU:OE1   | 8:L16:484:PRO:CG    | 2.18                     | 0.91              |
| 3:N16:1:MET:CB      | 3:N16:302:PRO:C     | 2.43                     | 0.91              |
| 5:P:16:PHE:CD1      | 6:O:311:LEU:CD1     | 2.54                     | 0.91              |
| 5:P:592:SER:HG      | 5:P:598:LEU:HD13    | 1.33                     | 0.91              |
| 8:L16:1026:ARG:CD   | 9:K16:1284:MET:HG2  | 2.01                     | 0.91              |
| 10:C16:653:TYR:OH   | 10:C16:679:ARG:HB3  | 1.70                     | 0.91              |
| 10:C:407:LYS:CE     | 10:C:465:PHE:CE2    | 2.54                     | 0.91              |
| 10:C8:556:VAL:CG1   | 10:C8:565:ARG:NH2   | 2.34                     | 0.91              |
| 11:A16:703:ALA:HA   | 24:D16:1398:ARG:CD  | 2.00                     | 0.91              |
| 18:B8:750:GLU:OE1   | 18:B8:760:ARG:NH2   | 2.04                     | 0.91              |
| 18:B8:1772:HIS:HD2  | 18:B8:1878:GLU:OE2  | 1.51                     | 0.91              |
| 10:C32:1757:GLN:OE1 | 12:A48:136:LEU:CD2  | 2.19                     | 0.91              |
| 12:A48:603:ALA:O    | 12:A48:616:ARG:NH1  | 2.03                     | 0.91              |
| 3:N:19:MET:HE2      | 3:N:23:GLY:O        | 1.70                     | 0.90              |
| 3:N8:1:MET:CB       | 3:N8:302:PRO:C      | 2.43                     | 0.90              |
| 2:M16:231:ARG:HG3   | 2:M16:299:GLY:O     | 1.72                     | 0.90              |
| 6:O:82:LEU:CD2      | 6:O:103:MET:HE3     | 2.00                     | 0.90              |
| 7:Q16:221:TRP:CZ3   | 7:Q16:222:PHE:CE2   | 2.58                     | 0.90              |
| 9:K8:1085:TYR:HH    | 9:K8:1093:SER:HA    | 1.29                     | 0.90              |
| 10:C16:847:ARG:HH21 | 10:C16:910:SER:HB2  | 1.35                     | 0.90              |
| 14:W:586:ILE:CD1    | 15:J:569:ALA:CA     | 2.46                     | 0.90              |
| 11:A16:718:THR:HG23 | 24:D16:1398:ARG:NH1 | 1.85                     | 0.90              |
| 18:B8:603:PHE:HB2   | 18:B8:619:ARG:NH2   | 1.85                     | 0.90              |
| 18:B8:786:ASP:OD2   | 24:D32:1066:VAL:CA  | 2.18                     | 0.90              |
| 23:J32:686:MET:HE1  | 23:J32:694:ARG:NE   | 1.86                     | 0.90              |
| 2:M:377:ARG:HH12    | 2:M:477:ASP:HB3     | 1.23                     | 0.90              |
| 1:R8:909:GLN:HE21   | 24:D40:1361:ALA:HB2 | 1.35                     | 0.90              |
| 1:R8:1460:MET:HE2   | 1:R8:1463:GLN:OE1   | 1.71                     | 0.90              |
| 2:M8:417:ARG:NH2    | 8:L8:415:PHE:HE2    | 1.62                     | 0.90              |
| 3:N8:162:THR:HG23   | 3:N8:168:VAL:HG21   | 1.53                     | 0.90              |
| 2:M16:672:TYR:HB2   | 2:M16:680:LYS:CD    | 2.01                     | 0.90              |
| 6:O8:54:VAL:HG13    | 6:O8:85:TRP:HE1     | 1.32                     | 0.90              |
| 6:O16:82:LEU:CD2    | 6:O16:103:MET:HE3   | 2.00                     | 0.90              |
| 9:K:1117:LEU:HG     | 9:K:1139:ILE:HD11   | 1.51                     | 0.90              |
| 10:C16:1466:ARG:HA  | 10:C16:1469:HIS:HE1 | 1.32                     | 0.90              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:1626:GLN:HE21 | 10:C16:1692:LYS:NZ  | 1.70                     | 0.90              |
| 10:C:345:MET:HE2     | 10:C:401:ILE:HD11   | 1.52                     | 0.90              |
| 10:C:1163:LEU:HD23   | 10:C:1166:SER:CB    | 2.00                     | 0.90              |
| 11:A16:326:TYR:HD1   | 17:F8:77:TYR:HB3    | 1.35                     | 0.90              |
| 19:48:250:ILE:HD13   | 20:E8:165:ARG:NH2   | 1.86                     | 0.90              |
| 21:H:322:LEU:HB3     | 22:I:300:LEU:HD11   | 0.90                     | 0.90              |
| 10:C32:1010:ALA:CA   | 10:C32:1192:ARG:NH2 | 2.33                     | 0.90              |
| 1:R8:1449:TRP:HZ3    | 2:M8:160:LEU:HD12   | 1.23                     | 0.90              |
| 1:R16:1428:VAL:O     | 1:R16:1431:ARG:HG2  | 1.72                     | 0.90              |
| 2:M16:844:VAL:HG21   | 4:T16:660:LEU:CD2   | 1.91                     | 0.90              |
| 5:P:55:ARG:HH12      | 5:P:64:ASP:HB2      | 1.27                     | 0.90              |
| 11:A24:326:TYR:HD1   | 17:F:77:TYR:HB3     | 1.35                     | 0.90              |
| 11:A24:748:GLU:OE1   | 24:D8:1398:ARG:NH1  | 2.05                     | 0.90              |
| 12:A:798:PHE:HE1     | 12:A:847:ARG:NH1    | 1.64                     | 0.90              |
| 10:C:1251:PHE:HZ     | 10:C:1319:ARG:NH1   | 1.63                     | 0.90              |
| 18:B8:643:MET:CE     | 18:B8:711:CYS:HB3   | 2.00                     | 0.90              |
| 22:I8:171:MET:CE     | 23:J8:592:VAL:HG13  | 2.02                     | 0.90              |
| 21:H24:322:LEU:HB3   | 22:I24:300:LEU:HD11 | 0.90                     | 0.90              |
| 2:M:625:HIS:NE2      | 3:N:225:PRO:HA      | 1.85                     | 0.90              |
| 2:M:627:TYR:HE2      | 3:N:165:GLY:C       | 1.80                     | 0.90              |
| 1:R16:1269:LEU:CD1   | 5:P16:684:ARG:CD    | 2.49                     | 0.90              |
| 2:M16:762:LEU:HB2    | 2:M16:813:ASN:HD22  | 1.32                     | 0.90              |
| 5:P16:16:PHE:CD1     | 6:O16:311:LEU:CD1   | 2.54                     | 0.90              |
| 9:K8:1160:ARG:NH2    | 9:K8:1220:ASN:ND2   | 2.18                     | 0.90              |
| 10:C16:228:ARG:NH2   | 10:C16:277:SER:HB3  | 1.85                     | 0.90              |
| 14:W:645:HIS:ND1     | 14:W:649:LEU:HD12   | 1.85                     | 0.90              |
| 14:W:649:LEU:CD2     | 15:J:575:ILE:HD12   | 1.90                     | 0.90              |
| 11:A32:676:TYR:HE2   | 24:D32:1396:PRO:CD  | 1.83                     | 0.90              |
| 18:B:1772:HIS:HD2    | 18:B:1878:GLU:OE2   | 1.51                     | 0.90              |
| 22:I16:300:LEU:HD21  | 23:J16:689:LEU:HD21 | 1.53                     | 0.90              |
| 24:D:405:GLN:OE1     | 24:D16:10:ARG:NE    | 1.86                     | 0.90              |
| 1:R:1428:VAL:HG23    | 6:O:165:LYS:CE      | 2.02                     | 0.90              |
| 1:R16:1078:SER:OG    | 5:P16:713:LEU:HD21  | 1.62                     | 0.90              |
| 8:L16:173:ASP:CB     | 12:A48:783:PHE:CE1  | 2.55                     | 0.90              |
| 9:K8:1085:TYR:CD1    | 9:K8:1093:SER:HB2   | 2.05                     | 0.90              |
| 11:A24:629:LEU:C     | 11:A24:678:LYS:NZ   | 2.27                     | 0.90              |
| 10:C:988:GLN:NE2     | 10:C:1064:PHE:HE1   | 1.70                     | 0.90              |
| 18:B8:1028:LYS:NZ    | 18:B8:1092:GLU:OE2  | 2.03                     | 0.90              |
| 19:4:250:ILE:CG1     | 20:E:165:ARG:NH2    | 2.34                     | 0.90              |
| 21:H:193:LEU:HD21    | 21:H:195:GLN:HE21   | 1.34                     | 0.90              |
| 2:M:417:ARG:HG2      | 8:L:346:TRP:CH2     | 2.06                     | 0.90              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M8:851:LEU:CD2     | 4:T8:653:GLN:HG2    | 2.01                     | 0.90              |
| 5:P:179:TYR:CE1      | 5:P:437:GLY:CA      | 2.54                     | 0.90              |
| 6:O:317:GLU:OE1      | 6:O:320:THR:OG1     | 1.89                     | 0.90              |
| 5:P8:13:LEU:HB3      | 6:O8:308:GLN:OE1    | 1.72                     | 0.90              |
| 9:K:1201:LEU:HD22    | 9:K:1264:ALA:HB2    | 1.52                     | 0.90              |
| 10:C16:345:MET:HE2   | 10:C16:401:ILE:HD11 | 1.52                     | 0.90              |
| 11:A40:326:TYR:HD1   | 17:F16:77:TYR:HB3   | 1.35                     | 0.90              |
| 10:C:150:ASP:OD1     | 24:D:1404:GLY:HA2   | 1.72                     | 0.90              |
| 10:C:653:TYR:OH      | 10:C:679:ARG:HB3    | 1.70                     | 0.90              |
| 10:C8:1285:VAL:HG23  | 10:C8:1738:MET:HE1  | 1.52                     | 0.90              |
| 11:A32:91:GLU:CB     | 18:B8:1112:LYS:CE   | 2.35                     | 0.90              |
| 17:F16:74:ILE:HG22   | 17:F16:76:ASP:HB2   | 1.51                     | 0.90              |
| 12:A48:696:ILE:HD12  | 12:A48:728:ILE:HD12 | 1.53                     | 0.90              |
| 2:M:851:LEU:CD2      | 4:T:653:GLN:HG2     | 2.01                     | 0.90              |
| 2:M8:417:ARG:CZ      | 8:L8:415:PHE:CZ     | 2.55                     | 0.90              |
| 2:M8:816:ARG:NH1     | 2:M8:849:LEU:CB     | 2.24                     | 0.90              |
| 2:M16:414:GLY:CA     | 8:L16:401:LYS:HZ2   | 1.80                     | 0.90              |
| 2:M16:762:LEU:CB     | 2:M16:813:ASN:HD22  | 1.83                     | 0.90              |
| 6:O8:119:ARG:HH21    | 6:O8:182:GLU:HG2    | 1.25                     | 0.90              |
| 5:P16:55:ARG:HH12    | 5:P16:64:ASP:HB2    | 1.27                     | 0.90              |
| 8:L8:1069:LEU:HD11   | 9:K8:1086:VAL:HG11  | 1.53                     | 0.90              |
| 8:L16:173:ASP:CB     | 12:A48:783:PHE:HE1  | 1.84                     | 0.90              |
| 9:K:939:ARG:NH2      | 9:K:967:ASP:OD2     | 2.05                     | 0.90              |
| 9:K8:635:ALA:HB2     | 9:K8:655:GLN:CD     | 1.96                     | 0.90              |
| 10:C24:1466:ARG:HA   | 10:C24:1469:HIS:HE1 | 1.32                     | 0.90              |
| 10:C24:1626:GLN:HE21 | 10:C24:1692:LYS:NZ  | 1.70                     | 0.90              |
| 12:A:136:LEU:CD2     | 10:C:1757:GLN:OE1   | 2.19                     | 0.90              |
| 11:A32:706:SER:HB2   | 24:D32:1398:ARG:CD  | 1.99                     | 0.90              |
| 22:I16:171:MET:CE    | 23:J16:592:VAL:HG13 | 2.02                     | 0.90              |
| 12:A48:707:LEU:CG    | 12:A48:767:ARG:NH2  | 2.29                     | 0.90              |
| 2:M8:544:LEU:HD21    | 2:M8:586:ALA:CB     | 2.01                     | 0.90              |
| 5:P16:57:PRO:CB      | 6:O16:29:LEU:HD11   | 2.01                     | 0.90              |
| 9:K:1085:TYR:CD1     | 9:K:1093:SER:HB2    | 2.05                     | 0.90              |
| 11:A24:691:ALA:HB1   | 24:D8:1397:THR:HG21 | 1.51                     | 0.90              |
| 11:A40:696:ILE:HD12  | 11:A40:728:ILE:HD12 | 1.53                     | 0.90              |
| 13:V:745:LEU:CD1     | 15:J:557:ARG:HH12   | 1.85                     | 0.90              |
| 14:W:591:LEU:HD22    | 15:J:566:ASN:OD1    | 1.72                     | 0.90              |
| 11:A32:11:THR:HG21   | 22:I24:162:GLN:NE2  | 1.87                     | 0.90              |
| 22:I:171:MET:CE      | 23:J32:592:VAL:HG13 | 2.02                     | 0.90              |
| 22:I:300:LEU:HD21    | 23:J32:689:LEU:HD21 | 1.53                     | 0.90              |
| 22:I8:300:LEU:HD21   | 23:J8:689:LEU:HD21  | 1.53                     | 0.90              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:J24:686:MET:HE1   | 23:J24:694:ARG:NE    | 1.86                     | 0.90              |
| 21:H16:269:PHE:HD1   | 22:I16:205:ARG:HH12  | 0.96                     | 0.90              |
| 1:R:1175:TYR:HA      | 1:R:1177:TRP:HZ3     | 1.37                     | 0.90              |
| 1:R:1185:THR:CG2     | 24:D:1462:PHE:CZ     | 2.54                     | 0.90              |
| 1:R8:1265:PHE:HE2    | 1:R8:1269:LEU:HD11   | 1.36                     | 0.90              |
| 5:P:96:VAL:HG13      | 5:P:481:ILE:HD13     | 1.54                     | 0.90              |
| 6:O16:317:GLU:OE1    | 6:O16:320:THR:OG1    | 1.89                     | 0.90              |
| 10:C24:169:GLN:HA    | 10:C24:169:GLN:OE1   | 1.72                     | 0.90              |
| 10:C24:390:HIS:CB    | 10:C24:452:LEU:CG    | 2.22                     | 0.90              |
| 10:C24:565:ARG:HD3   | 10:C24:568:TRP:CZ3   | 2.07                     | 0.90              |
| 10:C8:1258:LEU:HA    | 10:C8:1323:LEU:HD12  | 1.54                     | 0.90              |
| 10:C8:1626:GLN:HE21  | 10:C8:1692:LYS:NZ    | 1.70                     | 0.90              |
| 18:B:50:THR:HG21     | 18:B:179:GLN:NE2     | 1.86                     | 0.90              |
| 21:H24:193:LEU:HD21  | 21:H24:195:GLN:HE21  | 1.34                     | 0.90              |
| 24:D40:839:GLU:CD    | 24:D40:971:HIS:CD2   | 2.49                     | 0.90              |
| 10:C32:169:GLN:HA    | 10:C32:169:GLN:OE1   | 1.72                     | 0.90              |
| 10:C32:1121:ILE:HG22 | 10:C32:1133:ILE:HD13 | 1.52                     | 0.90              |
| 5:P8:96:VAL:HG13     | 5:P8:481:ILE:HD13    | 1.54                     | 0.90              |
| 9:K:975:MET:HE1      | 9:K:1005:LEU:CD2     | 2.02                     | 0.90              |
| 10:C:228:ARG:NH2     | 10:C:277:SER:HB3     | 1.85                     | 0.90              |
| 10:C:847:ARG:HH21    | 10:C:910:SER:HB2     | 1.35                     | 0.90              |
| 10:C:1258:LEU:HA     | 10:C:1323:LEU:HD12   | 1.54                     | 0.90              |
| 10:C:1466:ARG:HA     | 10:C:1469:HIS:HE1    | 1.31                     | 0.90              |
| 11:A16:11:THR:HG21   | 22:I:162:GLN:NE2     | 1.87                     | 0.90              |
| 11:A32:33:LEU:HD21   | 22:I24:286:LEU:HD13  | 1.54                     | 0.90              |
| 11:A32:36:ASN:HD22   | 22:I24:293:LYS:NZ    | 1.68                     | 0.90              |
| 18:B:603:PHE:HB2     | 18:B:619:ARG:NH2     | 1.85                     | 0.90              |
| 2:M16:672:TYR:CD2    | 2:M16:680:LYS:CD     | 2.53                     | 0.89              |
| 6:O8:82:LEU:CD2      | 6:O8:103:MET:HE3     | 2.00                     | 0.89              |
| 7:Q8:297:VAL:HG11    | 7:Q8:301:ARG:CB      | 2.02                     | 0.89              |
| 9:K8:1201:LEU:HD22   | 9:K8:1264:ALA:HB2    | 1.51                     | 0.89              |
| 10:C16:1285:VAL:HG23 | 10:C16:1738:MET:HE2  | 1.46                     | 0.89              |
| 10:C16:1348:LEU:HD12 | 10:C16:1359:ILE:CD1  | 1.88                     | 0.89              |
| 10:C24:1074:LEU:HD21 | 18:B8:256:VAL:HA     | 1.52                     | 0.89              |
| 10:C24:1121:ILE:HG22 | 10:C24:1133:ILE:HD13 | 1.52                     | 0.89              |
| 11:A40:33:LEU:HD21   | 22:I16:286:LEU:HD13  | 1.54                     | 0.89              |
| 10:C:807:GLN:OE1     | 10:C:811:ILE:HG21    | 1.71                     | 0.89              |
| 10:C8:1250:ALA:HB2   | 10:C8:1309:ARG:NH1   | 1.87                     | 0.89              |
| 18:B:618:VAL:CG1     | 18:B:621:VAL:HG23    | 2.02                     | 0.89              |
| 22:I24:290:ASP:OD1   | 22:I24:293:LYS:CE    | 2.20                     | 0.89              |
| 24:D8:1330:ARG:HH12  | 24:D16:719:ARG:CB    | 1.85                     | 0.89              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1258:LEU:HA   | 10:C32:1323:LEU:HD12 | 1.54                     | 0.89              |
| 1:R:1428:VAL:O       | 1:R:1431:ARG:HG2     | 1.72                     | 0.89              |
| 2:M8:627:TYR:HB3     | 3:N8:167:LEU:CD1     | 2.01                     | 0.89              |
| 2:M16:851:LEU:CD2    | 4:T16:653:GLN:HG2    | 2.01                     | 0.89              |
| 5:P:15:LEU:HD23      | 6:O:309:SER:O        | 1.69                     | 0.89              |
| 6:O16:173:VAL:HG22   | 6:O16:189:LEU:CD1    | 2.02                     | 0.89              |
| 9:K8:1039:ASP:CG     | 9:K8:1096:LYS:NZ     | 2.31                     | 0.89              |
| 10:C16:1250:ALA:HB2  | 10:C16:1309:ARG:NH1  | 1.87                     | 0.89              |
| 10:C24:807:GLN:OE1   | 10:C24:811:ILE:HG21  | 1.71                     | 0.89              |
| 11:A40:11:THR:HG21   | 22:I16:162:GLN:NE2   | 1.87                     | 0.89              |
| 11:A40:103:GLU:CG    | 21:H16:323:TYR:HE2   | 1.84                     | 0.89              |
| 10:C8:988:GLN:NE2    | 10:C8:1064:PHE:HE1   | 1.70                     | 0.89              |
| 11:A16:121:GLN:HE22  | 18:B:1559:ALA:HA     | 1.37                     | 0.89              |
| 18:B:86:LYS:HG2      | 18:B:123:LEU:HD11    | 0.90                     | 0.89              |
| 18:B8:50:THR:HG21    | 18:B8:179:GLN:NE2    | 1.86                     | 0.89              |
| 18:B8:712:PRO:CB     | 18:B8:759:MET:CE     | 2.49                     | 0.89              |
| 20:E8:352:PHE:CD1    | 20:E8:451:ILE:HD13   | 2.07                     | 0.89              |
| 21:H:366:MET:CE      | 22:I:332:MET:CE      | 2.50                     | 0.89              |
| 10:C32:807:GLN:OE1   | 10:C32:811:ILE:HG21  | 1.71                     | 0.89              |
| 1:R8:982:GLU:HG3     | 24:D40:1436:ARG:NH2  | 1.87                     | 0.89              |
| 5:P:633:LEU:CD2      | 5:P:647:LEU:CD1      | 2.49                     | 0.89              |
| 6:O:173:VAL:HG22     | 6:O:189:LEU:CD1      | 2.02                     | 0.89              |
| 5:P8:16:PHE:HE1      | 6:O8:311:LEU:HD11    | 1.13                     | 0.89              |
| 9:K:1085:TYR:CZ      | 9:K:1093:SER:CA      | 2.47                     | 0.89              |
| 10:C16:1285:VAL:HG23 | 10:C16:1738:MET:HE1  | 1.52                     | 0.89              |
| 10:C24:1699:LYS:HZ1  | 23:J24:722:LEU:HD22  | 0.83                     | 0.89              |
| 11:A40:388:VAL:N     | 11:A40:459:ARG:NH1   | 2.20                     | 0.89              |
| 10:C:1285:VAL:HG23   | 10:C:1738:MET:HE1    | 1.52                     | 0.89              |
| 11:A32:121:GLN:HE22  | 18:B8:1559:ALA:HA    | 1.37                     | 0.89              |
| 22:I:290:ASP:OD1     | 22:I:293:LYS:CE      | 2.20                     | 0.89              |
| 22:I8:131:ARG:HG3    | 23:J8:557:ARG:HH21   | 1.25                     | 0.89              |
| 21:H24:366:MET:CE    | 22:I24:332:MET:CE    | 2.50                     | 0.89              |
| 23:J16:686:MET:HE1   | 23:J16:694:ARG:NE    | 1.86                     | 0.89              |
| 24:D:308:ASN:HD22    | 24:D16:753:ARG:NE    | 1.45                     | 0.89              |
| 2:M:162:ILE:HD11     | 2:M:213:LEU:HG       | 0.89                     | 0.89              |
| 3:N:116:ILE:HG23     | 3:N:177:TYR:CE1      | 2.08                     | 0.89              |
| 3:N:270:THR:OG1      | 3:N:272:ASN:OD1      | 1.89                     | 0.89              |
| 2:M16:351:ALA:CB     | 8:L16:219:ILE:CG2    | 2.50                     | 0.89              |
| 8:L8:601:HIS:HE1     | 8:L8:631:LEU:HB2     | 1.37                     | 0.89              |
| 9:K:919:MET:SD       | 9:K:938:PHE:HE2      | 1.91                     | 0.89              |
| 9:K8:975:MET:HE3     | 9:K8:989:VAL:CG1     | 2.01                     | 0.89              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 9:K8:1270:VAL:O      | 9:K8:1272:GLU:N     | 2.05                     | 0.89              |
| 11:A24:696:ILE:HD12  | 11:A24:728:ILE:HD12 | 1.53                     | 0.89              |
| 11:A40:362:ARG:HD2   | 11:A40:366:ARG:HH22 | 1.04                     | 0.89              |
| 13:V:835:GLU:HG2     | 15:J:648:TYR:OH     | 1.70                     | 0.89              |
| 10:C:452:LEU:C       | 10:C:452:LEU:HD12   | 1.97                     | 0.89              |
| 11:A16:706:SER:CB    | 24:D16:1398:ARG:HG2 | 2.03                     | 0.89              |
| 18:B8:1156:GLN:CA    | 18:B8:1382:LYS:NZ   | 2.30                     | 0.89              |
| 18:B8:1256:THR:HG21  | 24:D32:1238:GLU:CG  | 1.99                     | 0.89              |
| 19:4:250:ILE:HD13    | 20:E:165:ARG:NH2    | 1.86                     | 0.89              |
| 19:48:100:ILE:HG22   | 19:48:102:LEU:CG    | 2.01                     | 0.89              |
| 3:N8:19:MET:HE2      | 3:N8:23:GLY:O       | 1.70                     | 0.89              |
| 5:P16:214:LEU:CD2    | 5:P16:236:VAL:CG1   | 2.51                     | 0.89              |
| 9:K:958:MET:HE3      | 9:K:974:LEU:CD2     | 2.01                     | 0.89              |
| 10:C8:64:LEU:CD2     | 10:C8:96:ARG:HG3    | 2.02                     | 0.89              |
| 22:I24:300:LEU:HD21  | 23:J24:689:LEU:HD21 | 1.53                     | 0.89              |
| 10:C32:390:HIS:ND1   | 10:C32:452:LEU:CB   | 2.34                     | 0.89              |
| 1:R:771:SER:CB       | 24:D:1317:ARG:HD2   | 2.02                     | 0.89              |
| 2:M:342:VAL:HG12     | 2:M:343:MET:N       | 1.87                     | 0.89              |
| 2:M8:342:VAL:HG12    | 2:M8:343:MET:N      | 1.87                     | 0.89              |
| 5:P8:214:LEU:CD2     | 5:P8:236:VAL:CG1    | 2.51                     | 0.89              |
| 6:O8:119:ARG:HH21    | 6:O8:182:GLU:CG     | 1.86                     | 0.89              |
| 5:P16:592:SER:HG     | 5:P16:598:LEU:HD13  | 1.35                     | 0.89              |
| 10:C24:345:MET:HE3   | 10:C24:401:ILE:HD11 | 1.46                     | 0.89              |
| 22:I:289:LEU:HD23    | 22:I:296:ARG:HH22   | 1.34                     | 0.89              |
| 10:C32:228:ARG:NH2   | 10:C32:277:SER:HB3  | 1.85                     | 0.89              |
| 9:K:1006:GLY:HA3     | 9:K:1013:LEU:HD13   | 1.55                     | 0.89              |
| 9:K8:958:MET:HE3     | 9:K8:974:LEU:CD2    | 2.01                     | 0.89              |
| 10:C16:64:LEU:CD2    | 10:C16:96:ARG:HG3   | 2.02                     | 0.89              |
| 10:C:64:LEU:CD2      | 10:C:96:ARG:HG3     | 2.02                     | 0.89              |
| 10:C8:169:GLN:OE1    | 10:C8:169:GLN:HA    | 1.72                     | 0.89              |
| 10:C8:453:LEU:CD2    | 10:C8:459:LEU:CD2   | 2.15                     | 0.89              |
| 11:A16:112:ALA:HB1   | 18:B:1416:LYS:HZ1   | 1.34                     | 0.89              |
| 18:B:195:MET:CE      | 18:B:199:LEU:CD2    | 2.18                     | 0.89              |
| 20:E8:353:ILE:HD13   | 20:E8:413:PHE:CG    | 2.06                     | 0.89              |
| 10:C32:1348:LEU:HD12 | 10:C32:1359:ILE:CD1 | 1.88                     | 0.89              |
| 1:R16:1075:LYS:HE2   | 5:P16:713:LEU:O     | 1.72                     | 0.89              |
| 2:M16:627:TYR:CD1    | 3:N16:166:ALA:O     | 2.26                     | 0.89              |
| 3:N16:116:ILE:HG23   | 3:N16:177:TYR:CE1   | 2.08                     | 0.89              |
| 5:P:57:PRO:CB        | 6:O:29:LEU:HD11     | 2.01                     | 0.89              |
| 7:Q:297:VAL:HG11     | 7:Q:301:ARG:CB      | 2.02                     | 0.89              |
| 8:L16:177:ARG:HD3    | 12:A48:744:GLU:OE1  | 0.90                     | 0.89              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K:1270:VAL:O      | 9:K:1272:GLU:N       | 2.05                     | 0.89              |
| 10:C16:1699:LYS:HZ2 | 23:J32:722:LEU:CD2   | 1.81                     | 0.89              |
| 10:C16:1814:LYS:HZ3 | 23:J32:738:MET:CB    | 1.85                     | 0.89              |
| 11:A24:11:THR:HG21  | 22:I8:162:GLN:NE2    | 1.87                     | 0.89              |
| 11:A24:326:TYR:HE1  | 17:F:77:TYR:HB2      | 1.37                     | 0.89              |
| 10:C24:386:ASN:CB   | 10:C24:449:GLU:OE1   | 2.20                     | 0.89              |
| 10:C24:847:ARG:HH21 | 10:C24:910:SER:HB2   | 1.34                     | 0.89              |
| 10:C:565:ARG:HD3    | 10:C:568:TRP:CZ3     | 2.08                     | 0.89              |
| 10:C8:1285:VAL:CG2  | 10:C8:1738:MET:HE1   | 2.01                     | 0.89              |
| 11:A32:326:TYR:HD1  | 17:F24:77:TYR:CB     | 1.83                     | 0.89              |
| 18:B8:618:VAL:CG1   | 18:B8:621:VAL:HG23   | 2.02                     | 0.89              |
| 18:B8:690:TRP:CE3   | 18:B8:739:VAL:CG2    | 2.55                     | 0.89              |
| 19:4:65:LYS:O       | 19:4:66:ALA:C        | 2.04                     | 0.89              |
| 10:C32:988:GLN:NE2  | 10:C32:1064:PHE:HE1  | 1.70                     | 0.89              |
| 5:P:57:PRO:CB       | 6:O:29:LEU:HD12      | 1.99                     | 0.89              |
| 7:Q16:297:VAL:HG11  | 7:Q16:301:ARG:CB     | 2.02                     | 0.89              |
| 9:K8:1039:ASP:CG    | 9:K8:1096:LYS:HZ3    | 1.81                     | 0.89              |
| 10:C16:565:ARG:HD3  | 10:C16:568:TRP:CZ3   | 2.07                     | 0.89              |
| 10:C16:1074:LEU:CD1 | 10:C16:1075:ASP:OD1  | 2.18                     | 0.89              |
| 10:C16:1682:VAL:CG2 | 10:C16:1758:LEU:HD23 | 2.03                     | 0.89              |
| 10:C24:1285:VAL:CG2 | 10:C24:1738:MET:HE1  | 2.01                     | 0.89              |
| 11:A32:711:ARG:CZ   | 24:D32:1399:SER:H    | 1.79                     | 0.89              |
| 18:B:816:LEU:HD23   | 18:B:822:ILE:HD13    | 1.54                     | 0.89              |
| 1:R:1425:PRO:CA     | 6:O:165:LYS:HZ1      | 1.79                     | 0.89              |
| 2:M:399:THR:HG21    | 2:M:480:ARG:NH2      | 1.88                     | 0.89              |
| 2:M:816:ARG:NH1     | 2:M:849:LEU:C        | 2.31                     | 0.89              |
| 2:M8:544:LEU:CD2    | 2:M8:586:ALA:HB1     | 2.01                     | 0.89              |
| 2:M8:816:ARG:NH1    | 2:M8:849:LEU:C       | 2.31                     | 0.89              |
| 2:M16:342:VAL:HG12  | 2:M16:343:MET:N      | 1.87                     | 0.89              |
| 5:P:13:LEU:HB3      | 6:O:308:GLN:OE1      | 1.72                     | 0.89              |
| 5:P8:57:PRO:CB      | 6:O8:29:LEU:HD11     | 2.01                     | 0.89              |
| 6:O8:317:GLU:OE1    | 6:O8:320:THR:OG1     | 1.89                     | 0.89              |
| 5:P16:13:LEU:HB3    | 6:O16:308:GLN:OE1    | 1.72                     | 0.89              |
| 5:P16:96:VAL:HG13   | 5:P16:481:ILE:HD13   | 1.54                     | 0.89              |
| 11:A24:33:LEU:HD21  | 22:I8:286:LEU:HD13   | 1.54                     | 0.89              |
| 10:C24:228:ARG:NH2  | 10:C24:277:SER:HB3   | 1.85                     | 0.89              |
| 13:V:825:GLN:HA     | 14:W:707:LYS:NZ      | 1.88                     | 0.89              |
| 13:V:844:MET:HG2    | 10:C8:1502:ARG:HH22  | 1.12                     | 0.89              |
| 10:C8:390:HIS:NE2   | 10:C8:459:LEU:HD12   | 1.87                     | 0.89              |
| 18:B:690:TRP:CE3    | 18:B:739:VAL:CG2     | 2.55                     | 0.89              |
| 18:B:1156:GLN:CA    | 18:B:1382:LYS:NZ     | 2.30                     | 0.89              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:816:LEU:HD23   | 18:B8:822:ILE:HD13   | 1.54                     | 0.89              |
| 20:E:352:PHE:CD1     | 20:E:451:ILE:HD13    | 2.07                     | 0.89              |
| 24:D8:857:THR:HG23   | 24:D8:885:TYR:OH     | 1.73                     | 0.89              |
| 10:C32:1250:ALA:HB2  | 10:C32:1309:ARG:NH1  | 1.88                     | 0.89              |
| 12:A48:388:VAL:N     | 12:A48:459:ARG:NH1   | 2.20                     | 0.89              |
| 2:M8:627:TYR:HE2     | 3:N8:162:THR:CG2     | 1.86                     | 0.88              |
| 6:O16:119:ARG:HH21   | 6:O16:182:GLU:CG     | 1.86                     | 0.88              |
| 9:K:1214:TYR:HB3     | 9:K:1269:CYS:SG      | 2.13                     | 0.88              |
| 11:A24:388:VAL:N     | 11:A24:459:ARG:NH1   | 2.20                     | 0.88              |
| 10:C24:847:ARG:CZ    | 10:C24:903:ASN:HB3   | 2.03                     | 0.88              |
| 10:C24:988:GLN:NE2   | 10:C24:1064:PHE:HE1  | 1.70                     | 0.88              |
| 10:C24:1285:VAL:HG23 | 10:C24:1738:MET:HE1  | 1.53                     | 0.88              |
| 11:A40:390:ALA:HB1   | 24:D32:1099:ARG:CD   | 2.03                     | 0.88              |
| 18:B:241:TYR:HB2     | 18:B:271:LEU:HD23    | 1.55                     | 0.88              |
| 18:B:928:ARG:NH2     | 18:B:969:ASP:O       | 2.05                     | 0.88              |
| 18:B8:113:TYR:CE1    | 18:B8:119:VAL:HG11   | 2.08                     | 0.88              |
| 1:R:1335:ILE:HG13    | 10:C:1170:VAL:CG2    | 2.02                     | 0.88              |
| 1:R8:983:ARG:O       | 24:D40:1360:ALA:HB2  | 1.72                     | 0.88              |
| 9:K8:1006:GLY:HA3    | 9:K8:1013:LEU:HD13   | 1.55                     | 0.88              |
| 10:C:1626:GLN:HE21   | 10:C:1692:LYS:NZ     | 1.70                     | 0.88              |
| 10:C8:1619:PRO:C     | 10:C8:1621:LYS:N     | 2.31                     | 0.88              |
| 11:A16:718:THR:CG2   | 24:D16:1398:ARG:HH12 | 1.87                     | 0.88              |
| 11:A32:696:ILE:HD12  | 11:A32:728:ILE:HD12  | 1.53                     | 0.88              |
| 18:B8:566:LYS:HE3    | 18:B8:574:GLU:OE2    | 1.72                     | 0.88              |
| 18:B8:779:LYS:HE2    | 18:B8:847:GLN:HE21   | 1.38                     | 0.88              |
| 19:48:109:GLN:O      | 19:48:418:LYS:HE2    | 1.73                     | 0.88              |
| 21:H8:366:MET:CE     | 22:I8:332:MET:CE     | 2.50                     | 0.88              |
| 10:C32:1626:GLN:HE21 | 10:C32:1692:LYS:NZ   | 1.70                     | 0.88              |
| 2:M16:399:THR:HG21   | 2:M16:480:ARG:NH2    | 1.88                     | 0.88              |
| 2:M16:816:ARG:NH1    | 2:M16:849:LEU:C      | 2.31                     | 0.88              |
| 6:O8:173:VAL:HG22    | 6:O8:189:LEU:CD1     | 2.02                     | 0.88              |
| 9:K:1074:ARG:NH1     | 9:K:1126:LEU:HD22    | 1.87                     | 0.88              |
| 9:K8:939:ARG:NH2     | 9:K8:967:ASP:OD2     | 2.05                     | 0.88              |
| 9:K8:1074:ARG:NH1    | 9:K8:1126:LEU:HD22   | 1.87                     | 0.88              |
| 10:C16:169:GLN:HA    | 10:C16:169:GLN:OE1   | 1.71                     | 0.88              |
| 10:C16:1699:LYS:HZ1  | 23:J32:722:LEU:HD22  | 0.73                     | 0.88              |
| 10:C:249:THR:C       | 10:C:251:GLY:H       | 1.75                     | 0.88              |
| 10:C:847:ARG:CZ      | 10:C:903:ASN:HB3     | 2.03                     | 0.88              |
| 11:A32:388:VAL:N     | 11:A32:459:ARG:NH1   | 2.20                     | 0.88              |
| 18:B8:241:TYR:HB2    | 18:B8:271:LEU:HD23   | 1.55                     | 0.88              |
| 20:E8:432:ILE:CB     | 24:D40:72:GLU:HG2    | 2.03                     | 0.88              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I:131:ARG:CG      | 23:J32:557:ARG:HH21  | 1.80                     | 0.88              |
| 22:I24:171:MET:CE    | 23:J24:592:VAL:HG13  | 2.02                     | 0.88              |
| 10:C32:64:LEU:CD2    | 10:C32:96:ARG:HG3    | 2.02                     | 0.88              |
| 3:N8:270:THR:OG1     | 3:N8:272:ASN:OD1     | 1.89                     | 0.88              |
| 8:L16:1026:ARG:HD2   | 9:K16:1284:MET:CB    | 2.04                     | 0.88              |
| 9:K8:1214:TYR:HB3    | 9:K8:1269:CYS:SG     | 2.13                     | 0.88              |
| 10:C16:1121:ILE:HG22 | 10:C16:1133:ILE:HD13 | 1.52                     | 0.88              |
| 11:A24:465:SER:HB3   | 24:D16:1100:GLN:NE2  | 1.87                     | 0.88              |
| 10:C24:390:HIS:CA    | 10:C24:452:LEU:HG    | 2.03                     | 0.88              |
| 10:C24:1547:LYS:CE   | 24:D24:1405:GLY:H    | 1.85                     | 0.88              |
| 12:A:388:VAL:N       | 12:A:459:ARG:NH1     | 2.20                     | 0.88              |
| 11:A16:33:LEU:HD21   | 22:I:286:LEU:HD13    | 1.54                     | 0.88              |
| 11:A16:326:TYR:HE1   | 17:F8:77:TYR:HB2     | 1.36                     | 0.88              |
| 18:B8:195:MET:HE2    | 18:B8:199:LEU:HD21   | 1.53                     | 0.88              |
| 18:B8:685:SER:C      | 18:B8:687:SER:N      | 2.31                     | 0.88              |
| 20:E8:432:ILE:CG2    | 24:D40:72:GLU:CD     | 2.43                     | 0.88              |
| 10:C32:1682:VAL:CG2  | 10:C32:1758:LEU:HD23 | 2.03                     | 0.88              |
| 3:N8:116:ILE:HG23    | 3:N8:177:TYR:CE1     | 2.08                     | 0.88              |
| 2:M16:540:TYR:HD1    | 2:M16:555:LEU:CD2    | 1.59                     | 0.88              |
| 9:K:1051:GLU:C       | 9:K:1053:MET:N       | 2.30                     | 0.88              |
| 9:K:1180:TRP:HZ2     | 9:K:1206:LEU:HD12    | 1.39                     | 0.88              |
| 10:C16:667:ILE:CD1   | 10:C16:670:GLU:O     | 2.22                     | 0.88              |
| 10:C16:962:PHE:CE2   | 10:C16:997:ILE:CD1   | 2.56                     | 0.88              |
| 10:C24:168:ARG:NH1   | 10:C24:229:PRO:HA    | 1.88                     | 0.88              |
| 10:C24:390:HIS:ND1   | 10:C24:452:LEU:CB    | 2.36                     | 0.88              |
| 12:A:440:LEU:HB3     | 12:A:443:LEU:CD1     | 2.04                     | 0.88              |
| 11:A16:388:VAL:N     | 11:A16:459:ARG:NH1   | 2.20                     | 0.88              |
| 11:A16:696:ILE:HD12  | 11:A16:728:ILE:HD12  | 1.53                     | 0.88              |
| 18:B:751:TYR:HH      | 18:B:804:ARG:HH12    | 1.20                     | 0.88              |
| 18:B:783:LYS:HE3     | 24:D16:1064:GLY:CA   | 2.02                     | 0.88              |
| 18:B8:86:LYS:HG2     | 18:B8:123:LEU:HD11   | 0.90                     | 0.88              |
| 18:B8:751:TYR:HH     | 18:B8:804:ARG:HH12   | 1.20                     | 0.88              |
| 19:4:153:ARG:HH21    | 20:E:467:ILE:HD11    | 1.39                     | 0.88              |
| 10:C32:1530:PHE:CE1  | 12:A48:132:MET:HE2   | 2.09                     | 0.88              |
| 1:R:1428:VAL:HG21    | 6:O:165:LYS:HE3      | 0.90                     | 0.88              |
| 1:R8:1185:THR:CG2    | 24:D40:1462:PHE:CZ   | 2.56                     | 0.88              |
| 1:R8:1428:VAL:O      | 1:R8:1431:ARG:HG2    | 1.72                     | 0.88              |
| 2:M16:417:ARG:HD2    | 8:L16:298:PHE:HD2    | 1.37                     | 0.88              |
| 5:P:109:ILE:CB       | 14:W:18:PRO:HG2      | 2.03                     | 0.88              |
| 5:P:214:LEU:CD2      | 5:P:236:VAL:CG1      | 2.51                     | 0.88              |
| 10:C16:1449:GLU:CD   | 24:D8:1151:SER:HA    | 1.98                     | 0.88              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1250:ALA:HB2 | 10:C24:1309:ARG:NH1  | 1.88                     | 0.88              |
| 11:A40:326:TYR:HE1  | 17:F16:77:TYR:HB2    | 1.37                     | 0.88              |
| 14:W:554:LYS:HD2    | 14:W:597:ARG:HH21    | 1.36                     | 0.88              |
| 10:C8:556:VAL:HG12  | 10:C8:565:ARG:CZ     | 2.04                     | 0.88              |
| 10:C8:847:ARG:HH21  | 10:C8:910:SER:HB2    | 1.35                     | 0.88              |
| 18:B:195:MET:HE2    | 18:B:199:LEU:HD21    | 1.53                     | 0.88              |
| 18:B:566:LYS:HE3    | 18:B:574:GLU:OE2     | 1.72                     | 0.88              |
| 18:B:1072:LEU:HD23  | 18:B:1076:GLU:OE2    | 1.73                     | 0.88              |
| 18:B8:1291:LEU:HD12 | 18:B8:1332:VAL:HG21  | 1.53                     | 0.88              |
| 22:I16:290:ASP:OD1  | 22:I16:293:LYS:CE    | 2.20                     | 0.88              |
| 24:D:1102:VAL:HG22  | 24:D:1153:GLN:OE1    | 1.73                     | 0.88              |
| 10:C32:168:ARG:NH1  | 10:C32:229:PRO:HA    | 1.88                     | 0.88              |
| 1:R:1460:MET:HE2    | 1:R:1463:GLN:OE1     | 1.71                     | 0.88              |
| 2:M:185:ARG:NH1     | 2:M:213:LEU:HD11     | 1.86                     | 0.88              |
| 10:C24:962:PHE:CE2  | 10:C24:997:ILE:CD1   | 2.56                     | 0.88              |
| 10:C24:1619:PRO:C   | 10:C24:1621:LYS:N    | 2.31                     | 0.88              |
| 14:W:711:ARG:NH1    | 10:C8:1606:GLY:C     | 2.32                     | 0.88              |
| 10:C:1682:VAL:CG2   | 10:C:1758:LEU:HD23   | 2.03                     | 0.88              |
| 18:B:113:TYR:CE1    | 18:B:119:VAL:HG11    | 2.08                     | 0.88              |
| 18:B8:94:LEU:HD21   | 18:B8:132:LEU:HD23   | 1.54                     | 0.88              |
| 18:B8:928:ARG:NH2   | 18:B8:969:ASP:O      | 2.06                     | 0.88              |
| 18:B8:1419:LYS:HG3  | 18:B8:1468:PHE:HE1   | 1.33                     | 0.88              |
| 20:E:429:PRO:N      | 24:D:72:GLU:OE2      | 2.04                     | 0.88              |
| 24:D:409:LEU:HD22   | 24:D16:746:ALA:H     | 1.37                     | 0.88              |
| 6:O:179:LYS:CG      | 6:O:183:GLN:OE1      | 2.22                     | 0.88              |
| 10:C16:1619:PRO:C   | 10:C16:1621:LYS:N    | 2.31                     | 0.88              |
| 10:C:1250:ALA:HB2   | 10:C:1309:ARG:NH1    | 1.87                     | 0.88              |
| 10:C8:168:ARG:NH1   | 10:C8:229:PRO:HA     | 1.88                     | 0.88              |
| 10:C8:345:MET:HE3   | 10:C8:401:ILE:HD11   | 1.46                     | 0.88              |
| 10:C8:960:PHE:CE1   | 10:C8:1138:GLU:HB2   | 2.09                     | 0.88              |
| 18:B:1725:THR:HG23  | 18:B:1830:LEU:CD2    | 2.02                     | 0.88              |
| 10:C32:962:PHE:CZ   | 10:C32:997:ILE:CD1   | 2.57                     | 0.88              |
| 2:M8:399:THR:HG21   | 2:M8:480:ARG:NH2     | 1.88                     | 0.88              |
| 3:N16:162:THR:HG23  | 3:N16:168:VAL:HG21   | 1.53                     | 0.88              |
| 8:L:346:TRP:CZ3     | 8:L:350:THR:HG21     | 2.09                     | 0.88              |
| 10:C16:1285:VAL:CG2 | 10:C16:1738:MET:HE1  | 2.01                     | 0.88              |
| 11:A24:362:ARG:HD2  | 11:A24:366:ARG:HH22  | 1.04                     | 0.88              |
| 10:C24:1258:LEU:HA  | 10:C24:1323:LEU:HD12 | 1.54                     | 0.88              |
| 13:V:850:LEU:HD23   | 15:J:665:ILE:HD12    | 1.54                     | 0.88              |
| 14:W:781:LEU:HD21   | 15:J:695:ILE:CG2     | 2.03                     | 0.88              |
| 18:B8:1072:LEU:HD23 | 18:B8:1076:GLU:OE2   | 1.73                     | 0.88              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 21:H16:366:MET:CE    | 22:I16:332:MET:CE    | 2.50                     | 0.88              |
| 10:C32:448:LYS:O     | 10:C32:450:PRO:HD3   | 1.74                     | 0.88              |
| 10:C32:847:ARG:CZ    | 10:C32:903:ASN:HB3   | 2.03                     | 0.88              |
| 10:C32:962:PHE:CE2   | 10:C32:997:ILE:CD1   | 2.56                     | 0.88              |
| 10:C32:1619:PRO:C    | 10:C32:1621:LYS:N    | 2.31                     | 0.88              |
| 10:C32:1686:LEU:HD23 | 10:C32:1810:LEU:HD21 | 1.56                     | 0.88              |
| 2:M16:417:ARG:HD3    | 8:L16:298:PHE:HD2    | 0.88                     | 0.88              |
| 10:C16:448:LYS:O     | 10:C16:450:PRO:HD3   | 1.74                     | 0.88              |
| 10:C:553:LEU:HD22    | 10:C:595:THR:HG21    | 1.56                     | 0.88              |
| 18:B:1291:LEU:HD12   | 18:B:1332:VAL:HG21   | 1.53                     | 0.88              |
| 2:M16:672:TYR:CG     | 2:M16:680:LYS:CE     | 2.57                     | 0.87              |
| 6:O:119:ARG:HH21     | 6:O:182:GLU:CG       | 1.86                     | 0.87              |
| 9:K8:847:LEU:HD21    | 9:K8:910:SER:HG      | 1.34                     | 0.87              |
| 10:C16:168:ARG:NH1   | 10:C16:229:PRO:HA    | 1.88                     | 0.87              |
| 10:C24:64:LEU:CD2    | 10:C24:96:ARG:HG3    | 2.02                     | 0.87              |
| 12:A:696:ILE:HD12    | 12:A:728:ILE:HD12    | 1.53                     | 0.87              |
| 22:I8:290:ASP:OD1    | 22:I8:293:LYS:CE     | 2.20                     | 0.87              |
| 2:M:738:ILE:HD11     | 2:M:779:SER:HB2      | 1.56                     | 0.87              |
| 3:N:43:ASN:HD22      | 10:C:503:THR:HG21    | 1.30                     | 0.87              |
| 1:R8:1175:TYR:HA     | 1:R8:1177:TRP:HZ3    | 1.37                     | 0.87              |
| 5:P:600:PHE:HE2      | 5:P:638:SER:OG       | 1.48                     | 0.87              |
| 7:Q8:124:PHE:CE1     | 7:Q8:125:TYR:OH      | 1.98                     | 0.87              |
| 8:L16:1034:VAL:CG2   | 8:L16:1068:PHE:HE2   | 1.83                     | 0.87              |
| 9:K16:792:LEU:HD11   | 9:K16:864:ILE:HD11   | 1.56                     | 0.87              |
| 10:C:663:ILE:O       | 10:C:667:ILE:N       | 2.07                     | 0.87              |
| 19:4:100:ILE:HG22    | 19:4:102:LEU:CG      | 2.01                     | 0.87              |
| 21:H16:322:LEU:HB3   | 22:I16:300:LEU:HD11  | 0.91                     | 0.87              |
| 24:D24:1330:ARG:NH2  | 24:D32:719:ARG:HH12  | 1.72                     | 0.87              |
| 10:C16:553:LEU:HD22  | 10:C16:595:THR:HG21  | 1.56                     | 0.87              |
| 10:C16:1530:PHE:CE1  | 11:A24:132:MET:HE2   | 2.09                     | 0.87              |
| 10:C24:962:PHE:CZ    | 10:C24:997:ILE:CD1   | 2.57                     | 0.87              |
| 11:A40:36:ASN:ND2    | 22:I16:293:LYS:NZ    | 2.23                     | 0.87              |
| 11:A40:468:VAL:HG22  | 24:D32:1103:LEU:HD12 | 0.89                     | 0.87              |
| 12:A:707:LEU:CG      | 12:A:767:ARG:NH2     | 2.29                     | 0.87              |
| 14:W:514:THR:N       | 14:W:607:ARG:HH12    | 1.71                     | 0.87              |
| 10:C:1619:PRO:C      | 10:C:1621:LYS:N      | 2.32                     | 0.87              |
| 11:A16:90:PHE:CB     | 18:B:1800:ARG:NH2    | 2.09                     | 0.87              |
| 11:A16:90:PHE:HB2    | 18:B:1788:ILE:HD13   | 0.88                     | 0.87              |
| 18:B8:90:ILE:HD13    | 18:B8:131:ILE:HG21   | 1.56                     | 0.87              |
| 18:B8:334:PHE:CZ     | 18:B8:338:ILE:HD11   | 2.10                     | 0.87              |
| 18:B8:514:THR:HG23   | 18:B8:549:TRP:CZ3    | 2.09                     | 0.87              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:690:TRP:HH2    | 18:B8:787:VAL:HG22   | 1.40                     | 0.87              |
| 12:A48:440:LEU:HB3   | 12:A48:443:LEU:CD1   | 2.04                     | 0.87              |
| 1:R:983:ARG:HD3      | 24:D:1364:PRO:HA     | 1.57                     | 0.87              |
| 3:N:162:THR:HG23     | 3:N:168:VAL:HG21     | 1.54                     | 0.87              |
| 10:C16:847:ARG:CZ    | 10:C16:903:ASN:HB3   | 2.03                     | 0.87              |
| 12:A:132:MET:HE2     | 10:C:1530:PHE:CE1    | 2.08                     | 0.87              |
| 10:C:1010:ALA:H      | 10:C:1192:ARG:HH22   | 0.88                     | 0.87              |
| 10:C8:878:ARG:NH2    | 10:C8:885:VAL:HG23   | 1.90                     | 0.87              |
| 10:C8:1348:LEU:HD12  | 10:C8:1359:ILE:CD1   | 1.88                     | 0.87              |
| 10:C8:1530:PHE:CE1   | 16:A8:132:MET:HE2    | 2.09                     | 0.87              |
| 11:A16:707:LEU:CG    | 11:A16:767:ARG:NH2   | 2.29                     | 0.87              |
| 18:B8:421:ASP:OD1    | 18:B8:468:ARG:NH1    | 2.06                     | 0.87              |
| 18:B8:1725:THR:HG23  | 18:B8:1830:LEU:CD2   | 2.02                     | 0.87              |
| 5:P:663:LEU:HB2      | 5:P:707:ASN:HD21     | 1.38                     | 0.87              |
| 5:P8:614:VAL:N       | 5:P8:629:ARG:NH2     | 2.22                     | 0.87              |
| 5:P8:614:VAL:CG2     | 5:P8:629:ARG:NH2     | 2.36                     | 0.87              |
| 10:C16:1258:LEU:HA   | 10:C16:1323:LEU:HD12 | 1.54                     | 0.87              |
| 10:C24:1682:VAL:CG2  | 10:C24:1758:LEU:HD23 | 2.03                     | 0.87              |
| 10:C:168:ARG:NH1     | 10:C:229:PRO:HA      | 1.88                     | 0.87              |
| 10:C8:553:LEU:HD22   | 10:C8:595:THR:HG21   | 1.56                     | 0.87              |
| 10:C8:1010:ALA:H     | 10:C8:1192:ARG:HH22  | 0.88                     | 0.87              |
| 18:B:1110:LEU:HD13   | 21:H:323:TYR:CZ      | 2.10                     | 0.87              |
| 18:B:1215:PHE:CE1    | 18:B:1234:MET:SD     | 2.68                     | 0.87              |
| 20:E:353:ILE:HG21    | 20:E:413:PHE:CD2     | 2.08                     | 0.87              |
| 2:M8:844:VAL:HG21    | 4:T8:660:LEU:CD2     | 1.91                     | 0.87              |
| 6:O16:119:ARG:HH21   | 6:O16:182:GLU:CA     | 1.87                     | 0.87              |
| 9:K8:1051:GLU:C      | 9:K8:1053:MET:N      | 2.30                     | 0.87              |
| 10:C16:1686:LEU:HD23 | 10:C16:1810:LEU:HD21 | 1.56                     | 0.87              |
| 10:C24:878:ARG:NH2   | 10:C24:885:VAL:HG23  | 1.90                     | 0.87              |
| 10:C8:1682:VAL:CG2   | 10:C8:1758:LEU:HD23  | 2.03                     | 0.87              |
| 18:B:421:ASP:OD1     | 18:B:468:ARG:NH1     | 2.06                     | 0.87              |
| 18:B:690:TRP:HH2     | 18:B:787:VAL:HG22    | 1.40                     | 0.87              |
| 10:C32:878:ARG:NH2   | 10:C32:885:VAL:HG23  | 1.90                     | 0.87              |
| 1:R8:1112:LYS:HD3    | 5:P8:712:PHE:HE1     | 1.37                     | 0.87              |
| 5:P8:175:MET:HE1     | 5:P8:436:ALA:HB2     | 1.57                     | 0.87              |
| 11:A24:36:ASN:ND2    | 22:I8:293:LYS:NZ     | 2.23                     | 0.87              |
| 10:C24:448:LYS:O     | 10:C24:450:PRO:HD3   | 1.74                     | 0.87              |
| 10:C24:667:ILE:CD1   | 10:C24:670:GLU:O     | 2.21                     | 0.87              |
| 10:C24:1686:LEU:HD23 | 10:C24:1810:LEU:HD21 | 1.56                     | 0.87              |
| 10:C:1271:PHE:HZ     | 10:C:1284:ASP:CG     | 1.75                     | 0.87              |
| 10:C:1285:VAL:CG2    | 10:C:1738:MET:HE1    | 2.01                     | 0.87              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A16:388:VAL:HG23  | 11:A16:459:ARG:HH12  | 1.40                     | 0.87              |
| 11:A32:326:TYR:HE1   | 17:F24:77:TYR:HB2    | 1.37                     | 0.87              |
| 18:B:90:ILE:HD13     | 18:B:131:ILE:HG21    | 1.56                     | 0.87              |
| 18:B8:1210:CYS:HG    | 18:B8:1234:MET:HE1   | 1.09                     | 0.87              |
| 21:H:316:ILE:O       | 21:H:318:ALA:N       | 2.08                     | 0.87              |
| 21:H8:322:LEU:HB3    | 22:I8:300:LEU:HD11   | 0.90                     | 0.87              |
| 2:M:820:LEU:HD13     | 2:M:820:LEU:O        | 1.75                     | 0.87              |
| 5:P16:57:PRO:CB      | 6:O16:29:LEU:HD12    | 2.00                     | 0.87              |
| 8:L8:977:PRO:HD2     | 9:K8:1004:ARG:HD2    | 1.55                     | 0.87              |
| 9:K:916:LYS:CG       | 9:K:919:MET:HE1      | 2.04                     | 0.87              |
| 10:C16:670:GLU:HG2   | 10:C16:671:LYS:HG3   | 1.56                     | 0.87              |
| 11:A24:388:VAL:HG23  | 11:A24:459:ARG:HH12  | 1.40                     | 0.87              |
| 10:C24:1548:ILE:HD11 | 24:D24:1407:PHE:HZ   | 1.11                     | 0.87              |
| 14:W:631:TYR:CZ      | 15:J:554:LEU:CD2     | 2.58                     | 0.87              |
| 10:C8:663:ILE:O      | 10:C8:667:ILE:N      | 2.07                     | 0.87              |
| 18:B:94:LEU:HD21     | 18:B:132:LEU:HD23    | 1.54                     | 0.87              |
| 18:B:334:PHE:CZ      | 18:B:338:ILE:HD11    | 2.09                     | 0.87              |
| 18:B8:1110:LEU:HD23  | 21:H24:326:GLY:CA    | 1.96                     | 0.87              |
| 20:E:353:ILE:HG21    | 20:E:413:PHE:HE2     | 1.29                     | 0.87              |
| 21:H8:316:ILE:O      | 21:H8:318:ALA:N      | 2.08                     | 0.87              |
| 12:A48:440:LEU:HB3   | 12:A48:443:LEU:HD12  | 1.57                     | 0.87              |
| 2:M8:162:ILE:HD11    | 2:M8:213:LEU:HG      | 0.89                     | 0.87              |
| 9:K:1139:ILE:O       | 9:K:1140:GLN:O       | 1.93                     | 0.87              |
| 10:C16:663:ILE:O     | 10:C16:667:ILE:N     | 2.07                     | 0.87              |
| 10:C16:962:PHE:CZ    | 10:C16:997:ILE:CD1   | 2.57                     | 0.87              |
| 12:A:440:LEU:HD13    | 12:A:443:LEU:HD11    | 1.57                     | 0.87              |
| 11:A32:711:ARG:CZ    | 24:D32:1399:SER:N    | 2.34                     | 0.87              |
| 18:B:514:THR:HG23    | 18:B:549:TRP:CZ3     | 2.09                     | 0.87              |
| 18:B8:783:LYS:CE     | 24:D32:1064:GLY:HA2  | 2.03                     | 0.87              |
| 21:H16:316:ILE:O     | 21:H16:318:ALA:N     | 2.08                     | 0.87              |
| 1:R:1033:LYS:HE3     | 24:D:1436:ARG:CZ     | 2.04                     | 0.86              |
| 2:M16:622:ARG:HB3    | 2:M16:624:ASP:OD1    | 1.75                     | 0.86              |
| 5:P:398:LYS:CB       | 5:P:426:MET:CE       | 2.43                     | 0.86              |
| 5:P:595:SER:O        | 5:P:597:GLY:N        | 2.08                     | 0.86              |
| 6:O8:119:ARG:HH21    | 6:O8:182:GLU:CA      | 1.87                     | 0.86              |
| 8:L:1041:SER:OG      | 8:L:1054:HIS:HE1     | 1.58                     | 0.86              |
| 10:C24:1530:PHE:CE1  | 11:A40:132:MET:HE2   | 2.09                     | 0.86              |
| 12:A:388:VAL:HG23    | 12:A:459:ARG:HH12    | 1.40                     | 0.86              |
| 10:C8:847:ARG:CZ     | 10:C8:903:ASN:HB3    | 2.03                     | 0.86              |
| 11:A16:36:ASN:ND2    | 22:I:293:LYS:NZ      | 2.23                     | 0.86              |
| 18:B8:782:THR:O      | 24:D32:1066:VAL:HG21 | 1.75                     | 0.86              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C32:663:ILE:O    | 10:C32:667:ILE:N     | 2.07                     | 0.86              |
| 1:R8:634:ARG:HD3    | 4:T8:160:HIS:HE1     | 1.39                     | 0.86              |
| 2:M16:416:VAL:CG1   | 8:L16:398:ALA:HB2    | 2.05                     | 0.86              |
| 9:K8:1051:GLU:C     | 9:K8:1053:MET:H      | 1.83                     | 0.86              |
| 10:C8:345:MET:HE2   | 10:C8:401:ILE:HD11   | 1.51                     | 0.86              |
| 10:C8:453:LEU:HD13  | 10:C8:486:LEU:CD2    | 2.06                     | 0.86              |
| 11:A32:36:ASN:ND2   | 22:I24:293:LYS:NZ    | 2.22                     | 0.86              |
| 11:A32:440:LEU:HD13 | 11:A32:443:LEU:HD11  | 1.57                     | 0.86              |
| 21:H24:316:ILE:O    | 21:H24:318:ALA:N     | 2.08                     | 0.86              |
| 10:C32:847:ARG:CZ   | 10:C32:911:ILE:H     | 1.89                     | 0.86              |
| 10:C32:1010:ALA:H   | 10:C32:1192:ARG:HH22 | 0.88                     | 0.86              |
| 5:P:152:ILE:CD1     | 14:W:762:GLN:HE22    | 1.86                     | 0.86              |
| 5:P:607:PHE:HE1     | 5:P:633:LEU:CD1      | 1.80                     | 0.86              |
| 5:P8:188:LEU:HD23   | 5:P8:380:MET:HE1     | 1.57                     | 0.86              |
| 5:P16:595:SER:O     | 5:P16:597:GLY:N      | 2.08                     | 0.86              |
| 10:C:169:GLN:HA     | 10:C:169:GLN:OE1     | 1.71                     | 0.86              |
| 10:C8:1265:ARG:O    | 10:C8:1268:ARG:HG3   | 1.75                     | 0.86              |
| 10:C8:1637:PHE:CE1  | 16:A8:136:LEU:HD11   | 2.10                     | 0.86              |
| 11:A32:206:VAL:CG1  | 11:A32:233:ALA:HB1   | 2.05                     | 0.86              |
| 18:B:685:SER:C      | 18:B:687:SER:N       | 2.31                     | 0.86              |
| 18:B8:345:GLU:HA    | 18:B8:351:MET:HE3    | 1.58                     | 0.86              |
| 18:B8:1439:LYS:HE2  | 24:D32:1257:ASN:HB2  | 1.54                     | 0.86              |
| 21:H:312:GLN:CG     | 21:H:316:ILE:CD1     | 2.39                     | 0.86              |
| 1:R:634:ARG:HD3     | 4:T:160:HIS:HE1      | 1.39                     | 0.86              |
| 4:T16:671:ILE:CD1   | 5:P16:698:GLY:C      | 2.49                     | 0.86              |
| 6:O:119:ARG:HH21    | 6:O:182:GLU:CA       | 1.87                     | 0.86              |
| 5:P8:112:LEU:HD13   | 5:P8:123:GLN:NE2     | 1.91                     | 0.86              |
| 5:P8:663:LEU:HB2    | 5:P8:707:ASN:HD21    | 1.38                     | 0.86              |
| 10:C16:878:ARG:NH2  | 10:C16:885:VAL:HG23  | 1.90                     | 0.86              |
| 10:C8:1285:VAL:HA   | 10:C8:1735:TYR:HE2   | 1.41                     | 0.86              |
| 18:B:816:LEU:HD23   | 18:B:822:ILE:CD1     | 2.05                     | 0.86              |
| 18:B8:313:ILE:CD1   | 18:B8:331:TRP:CD2    | 2.59                     | 0.86              |
| 19:4:100:ILE:HD11   | 19:4:274:PHE:HE1     | 1.41                     | 0.86              |
| 12:A48:362:ARG:HD2  | 12:A48:366:ARG:HH22  | 1.03                     | 0.86              |
| 2:M16:420:CYS:HB3   | 8:L16:391:TRP:CZ3    | 2.11                     | 0.86              |
| 2:M16:762:LEU:HB2   | 2:M16:813:ASN:HD21   | 0.90                     | 0.86              |
| 6:O8:179:LYS:CG     | 6:O8:183:GLN:OE1     | 2.22                     | 0.86              |
| 8:L16:1041:SER:OG   | 8:L16:1054:HIS:HE1   | 1.58                     | 0.86              |
| 9:K8:1180:TRP:HZ2   | 9:K8:1206:LEU:HD12   | 1.39                     | 0.86              |
| 11:A24:607:ARG:NH2  | 24:D16:914:PHE:HD1   | 1.72                     | 0.86              |
| 10:C24:663:ILE:HG22 | 10:C24:667:ILE:CD1   | 2.06                     | 0.86              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1285:VAL:HA  | 10:C24:1735:TYR:HE2  | 1.41                     | 0.86              |
| 14:W:638:VAL:CG1    | 15:J:561:PHE:CZ      | 2.58                     | 0.86              |
| 14:W:711:ARG:HD3    | 10:C8:1609:ASP:CG    | 1.99                     | 0.86              |
| 10:C:663:ILE:HG22   | 10:C:667:ILE:CD1     | 2.06                     | 0.86              |
| 18:B:345:GLU:HA     | 18:B:351:MET:HE3     | 1.58                     | 0.86              |
| 19:4:109:GLN:O      | 19:4:418:LYS:HE2     | 1.73                     | 0.86              |
| 22:I16:131:ARG:CD   | 23:J16:557:ARG:HH21  | 1.89                     | 0.86              |
| 12:A48:206:VAL:CG1  | 12:A48:233:ALA:HB1   | 2.05                     | 0.86              |
| 2:M:816:ARG:NH1     | 2:M:849:LEU:CB       | 2.24                     | 0.86              |
| 1:R8:1059:ILE:CG2   | 24:D40:1435:ARG:CZ   | 2.50                     | 0.86              |
| 5:P:322:CYS:HB3     | 13:V:767:GLU:OE2     | 1.76                     | 0.86              |
| 12:A:206:VAL:CG1    | 12:A:233:ALA:HB1     | 2.05                     | 0.86              |
| 2:M8:622:ARG:HB3    | 2:M8:624:ASP:OD1     | 1.75                     | 0.86              |
| 5:P:16:PHE:HE1      | 6:O:311:LEU:HD11     | 1.13                     | 0.86              |
| 5:P:398:LYS:HB2     | 5:P:426:MET:HE1      | 1.53                     | 0.86              |
| 5:P16:663:LEU:HB2   | 5:P16:707:ASN:HD21   | 1.38                     | 0.86              |
| 10:C16:1010:ALA:H   | 10:C16:1192:ARG:HH22 | 0.88                     | 0.86              |
| 10:C24:644:ASN:OD1  | 10:C24:679:ARG:NH2   | 2.08                     | 0.86              |
| 10:C:281:ASP:OD2    | 24:D:1398:ARG:CD     | 2.22                     | 0.86              |
| 10:C:667:ILE:CD1    | 10:C:670:GLU:O       | 2.22                     | 0.86              |
| 10:C:670:GLU:HG2    | 10:C:671:LYS:HG3     | 1.57                     | 0.86              |
| 10:C:854:LEU:HD23   | 10:C:911:ILE:HD11    | 1.58                     | 0.86              |
| 11:A16:122:LYS:CE   | 18:B:1757:GLU:CD     | 2.47                     | 0.86              |
| 11:A32:388:VAL:N    | 11:A32:459:ARG:HH12  | 1.73                     | 0.86              |
| 18:B:313:ILE:CD1    | 18:B:331:TRP:CD2     | 2.59                     | 0.86              |
| 19:4:286:TRP:CD1    | 20:E:163:ILE:HG23    | 2.10                     | 0.86              |
| 22:I:289:LEU:HD22   | 22:I:296:ARG:HH12    | 1.41                     | 0.86              |
| 21:H16:140:PRO:O    | 21:H16:165:ALA:HB2   | 1.76                     | 0.86              |
| 10:C32:553:LEU:HD22 | 10:C32:595:THR:HG21  | 1.56                     | 0.86              |
| 10:C32:586:PRO:HD2  | 10:C32:650:ARG:HH12  | 1.41                     | 0.86              |
| 1:R:1079:ASP:OD1    | 5:P:713:LEU:HD22     | 1.75                     | 0.86              |
| 1:R16:634:ARG:HD3   | 4:T16:160:HIS:HE1    | 1.38                     | 0.86              |
| 2:M16:820:LEU:HD13  | 2:M16:820:LEU:O      | 1.76                     | 0.86              |
| 5:P:188:LEU:HD23    | 5:P:380:MET:HE1      | 1.57                     | 0.86              |
| 5:P8:101:LEU:CD2    | 5:P8:133:TYR:CE2     | 2.58                     | 0.86              |
| 6:O16:179:LYS:CG    | 6:O16:183:GLN:OE1    | 2.22                     | 0.86              |
| 9:K:1230:LEU:HD23   | 9:K:1244:VAL:HG22    | 1.57                     | 0.86              |
| 10:C16:663:ILE:HG22 | 10:C16:667:ILE:CD1   | 2.06                     | 0.86              |
| 12:A:388:VAL:N      | 12:A:459:ARG:HH12    | 1.73                     | 0.86              |
| 10:C:1686:LEU:HD23  | 10:C:1810:LEU:HD21   | 1.56                     | 0.86              |
| 11:A16:206:VAL:CG1  | 11:A16:233:ALA:HB1   | 2.05                     | 0.86              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B8:457:SER:HA    | 18:B8:548:ARG:HH11   | 1.40                     | 0.86              |
| 18:B8:786:ASP:CG    | 24:D32:1066:VAL:CG1  | 2.35                     | 0.86              |
| 18:B8:1215:PHE:CE1  | 18:B8:1234:MET:SD    | 2.68                     | 0.86              |
| 18:B8:1248:LYS:NZ   | 18:B8:1253:ASP:OD1   | 2.08                     | 0.86              |
| 20:E8:353:ILE:HG21  | 20:E8:413:PHE:CD2    | 2.09                     | 0.86              |
| 21:H8:269:PHE:HD1   | 22:I8:205:ARG:HH12   | 0.96                     | 0.86              |
| 21:H8:366:MET:HE1   | 22:I8:332:MET:CE     | 2.06                     | 0.86              |
| 22:I8:131:ARG:CD    | 23:J8:557:ARG:HH21   | 1.89                     | 0.86              |
| 24:D:1013:HIS:NE2   | 24:D:1043:TYR:CE1    | 2.43                     | 0.86              |
| 10:C32:407:LYS:NZ   | 10:C32:465:PHE:HE2   | 1.74                     | 0.86              |
| 10:C32:453:LEU:HD13 | 10:C32:486:LEU:CD2   | 2.06                     | 0.86              |
| 10:C32:670:GLU:HG2  | 10:C32:671:LYS:HG3   | 1.56                     | 0.86              |
| 1:R:1425:PRO:HA     | 6:O:165:LYS:HZ3      | 1.04                     | 0.86              |
| 2:M8:738:ILE:HD11   | 2:M8:779:SER:HB2     | 1.56                     | 0.86              |
| 1:R16:1463:GLN:HA   | 6:O16:160:LEU:HD21   | 1.56                     | 0.86              |
| 2:M16:540:TYR:CE1   | 2:M16:555:LEU:HD21   | 1.97                     | 0.86              |
| 8:L16:856:LEU:HD23  | 9:K16:1281:SER:HB2   | 1.55                     | 0.86              |
| 9:K8:743:ARG:CZ     | 9:K8:772:TYR:CE1     | 2.58                     | 0.86              |
| 10:C16:1285:VAL:HA  | 10:C16:1735:TYR:HE2  | 1.41                     | 0.86              |
| 11:A40:440:LEU:HB3  | 11:A40:443:LEU:HD12  | 1.57                     | 0.86              |
| 10:C:35:ASN:CA      | 24:D:1148:LEU:HD11   | 2.04                     | 0.86              |
| 10:C:1348:LEU:HD12  | 10:C:1359:ILE:CD1    | 1.88                     | 0.86              |
| 11:A32:707:LEU:HB2  | 24:D32:1398:ARG:HH22 | 1.38                     | 0.86              |
| 18:B:1248:LYS:NZ    | 18:B:1253:ASP:OD1    | 2.08                     | 0.86              |
| 22:I16:289:LEU:HD22 | 22:I16:296:ARG:HH12  | 1.41                     | 0.86              |
| 24:D40:843:GLN:HE21 | 24:D40:971:HIS:CE1   | 1.94                     | 0.86              |
| 10:C32:1637:PHE:CE1 | 12:A48:136:LEU:HD11  | 2.10                     | 0.86              |
| 12:A48:440:LEU:HD13 | 12:A48:443:LEU:HD11  | 1.57                     | 0.86              |
| 2:M8:443:ARG:NH2    | 2:M8:461:GLU:OE1     | 2.09                     | 0.86              |
| 1:R16:1223:PHE:CE1  | 5:P16:676:GLN:NE2    | 2.43                     | 0.86              |
| 5:P:109:ILE:HD13    | 14:W:18:PRO:CG       | 2.04                     | 0.86              |
| 5:P8:467:GLN:HE21   | 6:O8:291:SER:HB3     | 1.39                     | 0.86              |
| 8:L16:945:ASN:O     | 9:K16:1282:SER:CB    | 2.23                     | 0.86              |
| 9:K8:1142:ARG:NH2   | 9:K8:1204:THR:HA     | 1.91                     | 0.86              |
| 10:C16:407:LYS:NZ   | 10:C16:465:PHE:HE2   | 1.74                     | 0.86              |
| 11:A24:206:VAL:CG1  | 11:A24:233:ALA:HB1   | 2.05                     | 0.86              |
| 10:C:878:ARG:NH2    | 10:C:885:VAL:HG23    | 1.90                     | 0.86              |
| 10:C8:670:GLU:HG2   | 10:C8:671:LYS:HG3    | 1.57                     | 0.86              |
| 10:C8:847:ARG:CZ    | 10:C8:911:ILE:H      | 1.88                     | 0.86              |
| 10:C8:1251:PHE:HZ   | 10:C8:1319:ARG:NH1   | 1.63                     | 0.86              |
| 18:B8:782:THR:O     | 24:D32:1066:VAL:CG2  | 2.22                     | 0.86              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1940:ALA:HB1   | 18:B8:1950:ILE:CD1   | 2.04                     | 0.86              |
| 19:48:286:TRP:CD1    | 20:E8:163:ILE:HG23   | 2.10                     | 0.86              |
| 21:H8:140:PRO:O      | 21:H8:165:ALA:HB2    | 1.76                     | 0.86              |
| 2:M:443:ARG:NH2      | 2:M:461:GLU:OE1      | 2.09                     | 0.85              |
| 2:M:622:ARG:HB3      | 2:M:624:ASP:OD1      | 1.75                     | 0.85              |
| 2:M16:844:VAL:HG22   | 4:T16:660:LEU:CD1    | 2.06                     | 0.85              |
| 5:P8:313:TRP:CZ2     | 5:P8:345:MET:HE2     | 2.11                     | 0.85              |
| 8:L:1074:ARG:HD2     | 9:K:1089:LYS:CB      | 2.06                     | 0.85              |
| 9:K8:635:ALA:HB2     | 9:K8:655:GLN:NE2     | 1.89                     | 0.85              |
| 10:C16:988:GLN:NE2   | 10:C16:1064:PHE:HE1  | 1.70                     | 0.85              |
| 11:A24:156:MET:HA    | 11:A24:555:HIS:HD2   | 1.38                     | 0.85              |
| 11:A24:388:VAL:N     | 11:A24:459:ARG:HH12  | 1.73                     | 0.85              |
| 10:C24:407:LYS:NZ    | 10:C24:465:PHE:HE2   | 1.74                     | 0.85              |
| 10:C24:663:ILE:O     | 10:C24:667:ILE:N     | 2.07                     | 0.85              |
| 10:C8:1686:LEU:HD23  | 10:C8:1810:LEU:HD21  | 1.56                     | 0.85              |
| 1:R:768:LEU:HD21     | 24:D:1313:LEU:HD21   | 1.56                     | 0.85              |
| 6:O8:119:ARG:NE      | 6:O8:181:GLU:O       | 2.09                     | 0.85              |
| 8:L8:1089:MET:HE3    | 9:K8:1000:SER:CB     | 2.05                     | 0.85              |
| 9:K:743:ARG:CZ       | 9:K:772:TYR:CE1      | 2.58                     | 0.85              |
| 10:C24:65:PRO:HG2    | 10:C24:96:ARG:HH22   | 1.42                     | 0.85              |
| 10:C24:1626:GLN:HE21 | 10:C24:1692:LYS:HZ3  | 1.20                     | 0.85              |
| 10:C8:1280:VAL:HG22  | 10:C8:1731:HIS:CE1   | 2.12                     | 0.85              |
| 10:C8:1703:ILE:HA    | 10:C8:1706:LEU:HD12  | 1.58                     | 0.85              |
| 11:A16:117:ILE:HG23  | 18:B:1516:THR:HG21   | 1.58                     | 0.85              |
| 18:B:313:ILE:HD13    | 18:B:331:TRP:CG      | 2.11                     | 0.85              |
| 18:B8:816:LEU:HD23   | 18:B8:822:ILE:CD1    | 2.05                     | 0.85              |
| 20:E:353:ILE:HD13    | 20:E:413:PHE:CG      | 2.06                     | 0.85              |
| 24:D40:1105:ALA:HB2  | 24:D40:1134:GLN:HE22 | 1.41                     | 0.85              |
| 10:C32:1285:VAL:CG2  | 10:C32:1738:MET:HE1  | 2.01                     | 0.85              |
| 12:A48:388:VAL:HG23  | 12:A48:459:ARG:HH12  | 1.40                     | 0.85              |
| 2:M16:185:ARG:NH1    | 2:M16:213:LEU:HD11   | 1.86                     | 0.85              |
| 2:M16:844:VAL:HG22   | 4:T16:660:LEU:HD11   | 1.56                     | 0.85              |
| 9:K:578:THR:HG23     | 9:K:616:ARG:HH22     | 0.68                     | 0.85              |
| 9:K:1039:ASP:CG      | 9:K:1096:LYS:NZ      | 2.31                     | 0.85              |
| 10:C16:186:LEU:HD22  | 10:C16:206:ARG:HG2   | 1.59                     | 0.85              |
| 13:V:783:TRP:CZ2     | 14:W:671:GLU:HA      | 2.11                     | 0.85              |
| 10:C:1280:VAL:HG22   | 10:C:1731:HIS:CE1    | 2.11                     | 0.85              |
| 10:C:1703:ILE:HA     | 10:C:1706:LEU:HD12   | 1.58                     | 0.85              |
| 10:C32:847:ARG:HH21  | 10:C32:910:SER:HB2   | 1.35                     | 0.85              |
| 1:R8:1265:PHE:HE2    | 5:P8:684:ARG:HD3     | 1.36                     | 0.85              |
| 2:M16:443:ARG:NH2    | 2:M16:461:GLU:OE1    | 2.09                     | 0.85              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P:467:GLN:HE21     | 6:O:291:SER:HB3      | 1.39                     | 0.85              |
| 8:L8:1041:SER:OG     | 8:L8:1054:HIS:HE1    | 1.58                     | 0.85              |
| 9:K:601:VAL:HG11     | 9:K:673:SER:HB3      | 1.56                     | 0.85              |
| 10:C16:1547:LYS:HZ3  | 24:D8:1405:GLY:CA    | 1.89                     | 0.85              |
| 10:C24:1637:PHE:CE1  | 11:A40:136:LEU:HD11  | 2.10                     | 0.85              |
| 12:A:136:LEU:HD11    | 10:C:1637:PHE:CE1    | 2.10                     | 0.85              |
| 10:C8:854:LEU:HD23   | 10:C8:911:ILE:HD11   | 1.58                     | 0.85              |
| 10:C8:960:PHE:CD2    | 10:C8:1138:GLU:HG2   | 2.11                     | 0.85              |
| 24:D:1099:ARG:NH2    | 24:D:1149:VAL:HG21   | 1.89                     | 0.85              |
| 2:M:625:HIS:CA       | 3:N:165:GLY:HA2      | 2.06                     | 0.85              |
| 2:M8:625:HIS:CA      | 3:N8:165:GLY:HA2     | 2.06                     | 0.85              |
| 5:P:322:CYS:CB       | 13:V:767:GLU:CD      | 2.49                     | 0.85              |
| 8:L8:608:PHE:CZ      | 8:L8:635:MET:CA      | 2.58                     | 0.85              |
| 10:C24:1121:ILE:CG2  | 10:C24:1133:ILE:HD13 | 2.07                     | 0.85              |
| 10:C:586:PRO:HD2     | 10:C:650:ARG:HH12    | 1.41                     | 0.85              |
| 11:A16:121:GLN:NE2   | 18:B:1559:ALA:CB     | 2.40                     | 0.85              |
| 18:B:1112:LYS:CE     | 21:H:327:SER:O       | 2.24                     | 0.85              |
| 18:B:1273:GLU:HG2    | 18:B:1276:LYS:HE3    | 0.93                     | 0.85              |
| 20:E8:123:CYS:SG     | 20:E8:135:ILE:HG21   | 2.17                     | 0.85              |
| 21:H:366:MET:HE1     | 22:I:332:MET:CE      | 2.06                     | 0.85              |
| 21:H24:366:MET:HE1   | 22:I24:332:MET:CE    | 2.06                     | 0.85              |
| 22:I24:131:ARG:CD    | 23:J24:557:ARG:HH21  | 1.89                     | 0.85              |
| 1:R:1033:LYS:CG      | 24:D:1436:ARG:HE     | 1.89                     | 0.85              |
| 2:M16:185:ARG:NH1    | 2:M16:213:LEU:HD12   | 1.91                     | 0.85              |
| 9:K8:578:THR:HG23    | 9:K8:616:ARG:HH22    | 0.68                     | 0.85              |
| 10:C16:1274:ALA:C    | 10:C16:1276:SER:H    | 1.84                     | 0.85              |
| 10:C16:1389:ILE:HD12 | 10:C16:1426:ARG:HH11 | 1.42                     | 0.85              |
| 10:C24:1010:ALA:H    | 10:C24:1192:ARG:HH22 | 0.88                     | 0.85              |
| 10:C24:1348:LEU:HD12 | 10:C24:1359:ILE:CD1  | 1.88                     | 0.85              |
| 10:C24:1699:LYS:HZ1  | 23:J24:722:LEU:CD2   | 1.71                     | 0.85              |
| 11:A40:388:VAL:N     | 11:A40:459:ARG:HH12  | 1.73                     | 0.85              |
| 13:V:814:MET:HE3     | 13:V:824:TRP:CH2     | 2.11                     | 0.85              |
| 10:C:453:LEU:HD13    | 10:C:486:LEU:CD2     | 2.06                     | 0.85              |
| 11:A16:706:SER:HB2   | 24:D16:1398:ARG:HD3  | 1.57                     | 0.85              |
| 18:B:712:PRO:CB      | 18:B:759:MET:CE      | 2.49                     | 0.85              |
| 18:B8:968:PHE:CE1    | 18:B8:998:LEU:HD23   | 2.12                     | 0.85              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:CA     | 2.53                     | 0.85              |
| 21:H24:140:PRO:O     | 21:H24:165:ALA:HB2   | 1.76                     | 0.85              |
| 10:C32:499:LEU:CD2   | 10:C32:505:PHE:CE2   | 2.60                     | 0.85              |
| 10:C32:1121:ILE:CG2  | 10:C32:1133:ILE:HD13 | 2.07                     | 0.85              |
| 5:P8:595:SER:O       | 5:P8:597:GLY:N       | 2.08                     | 0.85              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:1142:ARG:NH2     | 9:K:1204:THR:HA      | 1.91                     | 0.85              |
| 9:K8:1035:SER:HB3    | 9:K8:1088:ASP:OD2    | 1.77                     | 0.85              |
| 9:K8:1230:LEU:HD23   | 9:K8:1244:VAL:HG22   | 1.57                     | 0.85              |
| 10:C16:110:ARG:HH12  | 10:C16:118:LEU:HD11  | 1.41                     | 0.85              |
| 10:C16:644:ASN:OD1   | 10:C16:679:ARG:NH2   | 2.08                     | 0.85              |
| 10:C24:390:HIS:NE2   | 10:C24:449:GLU:CD    | 2.28                     | 0.85              |
| 10:C24:670:GLU:HG2   | 10:C24:671:LYS:HG3   | 1.56                     | 0.85              |
| 11:A40:206:VAL:CG1   | 11:A40:233:ALA:HB1   | 2.05                     | 0.85              |
| 10:C:627:VAL:HG12    | 10:C:628:GLY:N       | 1.91                     | 0.85              |
| 11:A32:440:LEU:HB3   | 11:A32:443:LEU:HD12  | 1.56                     | 0.85              |
| 18:B:1529:GLU:OE2    | 24:D16:1415:LEU:HG   | 1.73                     | 0.85              |
| 18:B8:1112:LYS:CE    | 21:H24:327:SER:C     | 2.48                     | 0.85              |
| 20:E:123:CYS:SG      | 20:E:135:ILE:HG21    | 2.17                     | 0.85              |
| 21:H16:366:MET:HE1   | 22:I16:332:MET:CE    | 2.06                     | 0.85              |
| 10:C32:854:LEU:HD23  | 10:C32:911:ILE:HD11  | 1.58                     | 0.85              |
| 2:M8:185:ARG:NH1     | 2:M8:213:LEU:HD11    | 1.86                     | 0.85              |
| 2:M8:844:VAL:HG22    | 4:T8:660:LEU:CD1     | 2.06                     | 0.85              |
| 2:M16:627:TYR:HE1    | 3:N16:162:THR:CB     | 1.90                     | 0.85              |
| 5:P16:179:TYR:OH     | 5:P16:436:ALA:O      | 1.93                     | 0.85              |
| 5:P16:188:LEU:HD23   | 5:P16:380:MET:HE1    | 1.58                     | 0.85              |
| 10:C16:450:PRO:HB3   | 10:C16:485:THR:O     | 1.77                     | 0.85              |
| 11:A24:288:HIS:HB2   | 11:A24:354:ARG:NH1   | 1.92                     | 0.85              |
| 11:A24:607:ARG:CZ    | 24:D16:914:PHE:CE1   | 2.60                     | 0.85              |
| 10:C24:453:LEU:HD13  | 10:C24:486:LEU:CD2   | 2.06                     | 0.85              |
| 10:C24:553:LEU:HD22  | 10:C24:595:THR:HG21  | 1.56                     | 0.85              |
| 10:C:150:ASP:OD1     | 24:D:1404:GLY:CA     | 2.25                     | 0.85              |
| 11:A32:121:GLN:NE2   | 18:B8:1559:ALA:CB    | 2.40                     | 0.85              |
| 11:A32:121:GLN:NE2   | 18:B8:1559:ALA:HA    | 1.91                     | 0.85              |
| 10:C32:1280:VAL:HG22 | 10:C32:1731:HIS:CE1  | 2.11                     | 0.85              |
| 1:R16:1175:TYR:HA    | 1:R16:1177:TRP:HZ3   | 1.38                     | 0.85              |
| 5:P8:57:PRO:CB       | 6:O8:29:LEU:HD12     | 2.00                     | 0.85              |
| 10:C24:110:ARG:HH12  | 10:C24:118:LEU:HD11  | 1.41                     | 0.85              |
| 11:A16:714:GLY:HA3   | 24:D16:1398:ARG:HH21 | 1.37                     | 0.85              |
| 11:A32:122:LYS:CE    | 18:B8:1757:GLU:CD    | 2.47                     | 0.85              |
| 11:A32:259:ILE:CG2   | 11:A32:276:LEU:HD22  | 2.07                     | 0.85              |
| 18:B8:313:ILE:HD13   | 18:B8:331:TRP:CG     | 2.11                     | 0.85              |
| 19:4:103:GLN:CD      | 19:4:411:LEU:HD13    | 2.01                     | 0.85              |
| 10:C16:1074:LEU:CD1  | 10:C16:1075:ASP:N    | 2.40                     | 0.85              |
| 11:A24:273:ARG:HE    | 11:A24:479:LEU:HD23  | 1.42                     | 0.85              |
| 10:C24:1439:ILE:HD12 | 10:C24:1457:LEU:HD13 | 1.58                     | 0.85              |
| 11:A16:259:ILE:CG2   | 11:A16:276:LEU:HD22  | 2.07                     | 0.85              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 22:I24:289:LEU:HD22  | 22:I24:296:ARG:HH12 | 1.41                     | 0.85              |
| 24:D24:857:THR:HG21  | 24:D24:889:LEU:HD13 | 1.56                     | 0.85              |
| 10:C32:1285:VAL:HA   | 10:C32:1735:TYR:HE2 | 1.41                     | 0.85              |
| 10:C32:1290:HIS:CD2  | 10:C32:1334:MET:CE  | 2.60                     | 0.85              |
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:HD13  | 1.75                     | 0.84              |
| 2:M:844:VAL:HG21     | 4:T:660:LEU:CD2     | 1.92                     | 0.84              |
| 2:M8:762:LEU:CB      | 2:M8:813:ASN:HD22   | 1.84                     | 0.84              |
| 6:O8:119:ARG:NH2     | 6:O8:182:GLU:CG     | 2.40                     | 0.84              |
| 5:P16:179:TYR:CE1    | 5:P16:437:GLY:N     | 2.42                     | 0.84              |
| 5:P16:467:GLN:HE21   | 6:O16:291:SER:HB3   | 1.39                     | 0.84              |
| 10:C16:1280:VAL:HG22 | 10:C16:1731:HIS:CE1 | 2.11                     | 0.84              |
| 10:C16:1290:HIS:CD2  | 10:C16:1334:MET:CE  | 2.60                     | 0.84              |
| 10:C16:1637:PHE:CE1  | 11:A24:136:LEU:HD11 | 2.10                     | 0.84              |
| 10:C24:389:LEU:HD21  | 10:C24:447:PHE:HE1  | 1.41                     | 0.84              |
| 15:J:722:LEU:HD22    | 10:C8:1623:ILE:HG12 | 1.58                     | 0.84              |
| 10:C8:1389:ILE:HD12  | 10:C8:1426:ARG:HH11 | 1.42                     | 0.84              |
| 10:C32:1466:ARG:HH12 | 12:A48:127:SER:CB   | 1.90                     | 0.84              |
| 12:A48:259:ILE:CG2   | 12:A48:276:LEU:HD22 | 2.07                     | 0.84              |
| 12:A48:798:PHE:HE1   | 12:A48:847:ARG:NH1  | 1.64                     | 0.84              |
| 2:M8:672:TYR:HB3     | 2:M8:680:LYS:HD2    | 0.85                     | 0.84              |
| 2:M16:162:ILE:HD11   | 2:M16:213:LEU:HG    | 0.89                     | 0.84              |
| 2:M16:622:ARG:NH2    | 2:M16:624:ASP:OD2   | 2.11                     | 0.84              |
| 2:M16:625:HIS:CA     | 3:N16:165:GLY:HA2   | 2.06                     | 0.84              |
| 10:C24:1265:ARG:O    | 10:C24:1268:ARG:CD  | 2.25                     | 0.84              |
| 10:C24:1274:ALA:C    | 10:C24:1276:SER:H   | 1.84                     | 0.84              |
| 10:C24:1280:VAL:HG22 | 10:C24:1731:HIS:CE1 | 2.11                     | 0.84              |
| 11:A40:288:HIS:HB2   | 11:A40:354:ARG:NH1  | 1.92                     | 0.84              |
| 14:W:739:ARG:HH22    | 15:J:664:GLN:HE21   | 1.15                     | 0.84              |
| 18:B:1940:ALA:HB1    | 18:B:1950:ILE:CD1   | 2.04                     | 0.84              |
| 18:B8:1045:LYS:NZ    | 18:B8:1100:LEU:CD2  | 2.41                     | 0.84              |
| 18:B8:1161:LEU:HD11  | 18:B8:1403:ILE:HG21 | 1.59                     | 0.84              |
| 18:B8:1575:GLN:NE2   | 24:D32:1403:LEU:CD2 | 2.18                     | 0.84              |
| 18:B8:1673:ARG:O     | 18:B8:1676:VAL:CG2  | 2.22                     | 0.84              |
| 19:48:103:GLN:CD     | 19:48:411:LEU:HD13  | 2.01                     | 0.84              |
| 22:I:131:ARG:CD      | 23:J32:557:ARG:HH21 | 1.89                     | 0.84              |
| 21:H24:228:LEU:HD11  | 23:J24:593:VAL:HG22 | 1.59                     | 0.84              |
| 10:C32:1265:ARG:O    | 10:C32:1268:ARG:HG3 | 1.75                     | 0.84              |
| 10:C24:1290:HIS:CD2  | 10:C24:1334:MET:CE  | 2.60                     | 0.84              |
| 10:C24:1424:GLN:NE2  | 10:C24:1478:VAL:CG1 | 2.40                     | 0.84              |
| 12:A:127:SER:CB      | 10:C:1466:ARG:HH12  | 1.90                     | 0.84              |
| 10:C:1290:HIS:CD2    | 10:C:1334:MET:CE    | 2.60                     | 0.84              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C8:499:LEU:CD2    | 10:C8:505:PHE:CE2    | 2.60                     | 0.84              |
| 10:C8:1466:ARG:HH12  | 16:A8:127:SER:CB     | 1.90                     | 0.84              |
| 11:A32:90:PHE:CD1    | 18:B8:1788:ILE:HG22  | 2.10                     | 0.84              |
| 11:A32:117:ILE:HG23  | 18:B8:1516:THR:HG21  | 1.58                     | 0.84              |
| 11:A32:718:THR:HG23  | 24:D32:1398:ARG:NH1  | 1.91                     | 0.84              |
| 18:B:1439:LYS:HD3    | 24:D16:1257:ASN:ND2  | 1.92                     | 0.84              |
| 18:B8:1155:ILE:O     | 18:B8:1159:SER:OG    | 1.94                     | 0.84              |
| 10:C32:389:LEU:CD2   | 10:C32:447:PHE:CE1   | 2.60                     | 0.84              |
| 2:M:622:ARG:NH2      | 2:M:624:ASP:OD2      | 2.11                     | 0.84              |
| 2:M8:534:HIS:HD2     | 2:M8:557:THR:HG22    | 1.40                     | 0.84              |
| 2:M16:628:LEU:CD1    | 3:N16:223:GLY:C      | 2.51                     | 0.84              |
| 3:N16:1:MET:HB2      | 3:N16:302:PRO:O      | 1.77                     | 0.84              |
| 3:N16:19:MET:CE      | 3:N16:23:GLY:O       | 2.25                     | 0.84              |
| 5:P8:101:LEU:HD23    | 5:P8:133:TYR:CE2     | 2.12                     | 0.84              |
| 9:K:635:ALA:HB2      | 9:K:655:GLN:NE2      | 1.88                     | 0.84              |
| 9:K8:955:TYR:OH      | 9:K8:985:PHE:N       | 2.11                     | 0.84              |
| 10:C16:854:LEU:HD23  | 10:C16:911:ILE:HD11  | 1.58                     | 0.84              |
| 10:C16:1074:LEU:HD11 | 10:C16:1075:ASP:CG   | 2.01                     | 0.84              |
| 10:C16:1424:GLN:NE2  | 10:C16:1478:VAL:CG1  | 2.40                     | 0.84              |
| 10:C24:186:LEU:HD22  | 10:C24:206:ARG:HG2   | 1.59                     | 0.84              |
| 10:C24:1708:ARG:NH2  | 21:H24:275:LYS:CG    | 2.09                     | 0.84              |
| 10:C:450:PRO:HB3     | 10:C:485:THR:O       | 1.77                     | 0.84              |
| 10:C8:1439:ILE:HD12  | 10:C8:1457:LEU:HD13  | 1.58                     | 0.84              |
| 11:A32:36:ASN:ND2    | 22:I24:293:LYS:HE2   | 1.92                     | 0.84              |
| 24:D:400:VAL:HB      | 24:D16:751:MET:HE3   | 1.57                     | 0.84              |
| 24:D32:642:VAL:CG2   | 24:D40:631:ARG:CZ    | 2.52                     | 0.84              |
| 1:R16:1223:PHE:CZ    | 5:P16:676:GLN:OE1    | 2.29                     | 0.84              |
| 2:M16:738:ILE:HD11   | 2:M16:779:SER:HB2    | 1.56                     | 0.84              |
| 6:O:119:ARG:NE       | 6:O:181:GLU:O        | 2.10                     | 0.84              |
| 6:O8:176:ASN:ND2     | 6:O8:179:LYS:HE3     | 1.93                     | 0.84              |
| 6:O16:119:ARG:NE     | 6:O16:181:GLU:O      | 2.09                     | 0.84              |
| 8:L16:173:ASP:OD2    | 12:A48:797:VAL:CG1   | 2.26                     | 0.84              |
| 9:K:847:LEU:CD2      | 9:K:910:SER:CB       | 2.55                     | 0.84              |
| 9:K:1051:GLU:C       | 9:K:1053:MET:H       | 1.83                     | 0.84              |
| 9:K8:847:LEU:CD2     | 9:K8:910:SER:CB      | 2.55                     | 0.84              |
| 10:C16:453:LEU:HD13  | 10:C16:486:LEU:CD2   | 2.06                     | 0.84              |
| 10:C16:1265:ARG:O    | 10:C16:1268:ARG:CD   | 2.26                     | 0.84              |
| 10:C24:1265:ARG:O    | 10:C24:1268:ARG:HG3  | 1.75                     | 0.84              |
| 10:C24:1389:ILE:HD12 | 10:C24:1426:ARG:HH11 | 1.42                     | 0.84              |
| 10:C24:1814:LYS:NZ   | 23:J24:738:MET:SD    | 2.51                     | 0.84              |
| 11:A40:388:VAL:HG23  | 11:A40:459:ARG:HH12  | 1.40                     | 0.84              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 14:W:711:ARG:HD3     | 10:C8:1609:ASP:CB    | 2.07                     | 0.84              |
| 10:C:186:LEU:HD22    | 10:C:206:ARG:HG2     | 1.58                     | 0.84              |
| 10:C:1121:ILE:CG2    | 10:C:1133:ILE:HD13   | 2.07                     | 0.84              |
| 11:A32:90:PHE:CB     | 18:B8:1788:ILE:HG21  | 2.06                     | 0.84              |
| 11:A32:388:VAL:HG23  | 11:A32:459:ARG:HH12  | 1.40                     | 0.84              |
| 11:A32:718:THR:CG2   | 24:D32:1398:ARG:HH12 | 1.90                     | 0.84              |
| 24:D:405:GLN:CA      | 24:D16:10:ARG:HH11   | 1.89                     | 0.84              |
| 10:C32:627:VAL:HG12  | 10:C32:628:GLY:N     | 1.91                     | 0.84              |
| 10:C32:1424:GLN:NE2  | 10:C32:1478:VAL:CG1  | 2.40                     | 0.84              |
| 12:A48:388:VAL:N     | 12:A48:459:ARG:HH12  | 1.73                     | 0.84              |
| 2:M8:399:THR:HG21    | 2:M8:480:ARG:HH21    | 1.40                     | 0.84              |
| 2:M8:820:LEU:HD13    | 2:M8:820:LEU:O       | 1.76                     | 0.84              |
| 1:R16:1463:GLN:HA    | 6:O16:160:LEU:CD2    | 2.07                     | 0.84              |
| 5:P16:313:TRP:CZ2    | 5:P16:345:MET:HE2    | 2.11                     | 0.84              |
| 8:L:1089:MET:CE      | 9:K:1000:SER:HB2     | 2.08                     | 0.84              |
| 10:C16:1439:ILE:HD12 | 10:C16:1457:LEU:HD13 | 1.58                     | 0.84              |
| 10:C16:1547:LYS:CD   | 24:D8:1406:SER:N     | 2.34                     | 0.84              |
| 11:A24:440:LEU:HB3   | 11:A24:443:LEU:HD12  | 1.57                     | 0.84              |
| 10:C24:1466:ARG:HH12 | 11:A40:127:SER:CB    | 1.90                     | 0.84              |
| 14:W:649:LEU:HD21    | 15:J:575:ILE:CD1     | 1.97                     | 0.84              |
| 10:C8:1121:ILE:CG2   | 10:C8:1133:ILE:HD13  | 2.06                     | 0.84              |
| 11:A16:440:LEU:HB3   | 11:A16:443:LEU:CD1   | 2.04                     | 0.84              |
| 18:B8:1112:LYS:HE3   | 21:H24:327:SER:HA    | 1.57                     | 0.84              |
| 20:E8:432:ILE:HD12   | 24:D40:72:GLU:CG     | 1.89                     | 0.84              |
| 21:H8:228:LEU:HD11   | 23:J8:593:VAL:HG22   | 1.59                     | 0.84              |
| 24:D24:1452:LYS:NZ   | 24:D32:971:HIS:CE1   | 2.46                     | 0.84              |
| 12:A48:288:HIS:HB2   | 12:A48:354:ARG:NH1   | 1.92                     | 0.84              |
| 1:R:634:ARG:CD       | 4:T:160:HIS:CE1      | 2.61                     | 0.84              |
| 2:M8:547:LYS:NZ      | 2:M8:554:PHE:CE1     | 2.46                     | 0.84              |
| 2:M8:844:VAL:HG22    | 4:T8:660:LEU:HD11    | 1.57                     | 0.84              |
| 8:L8:1074:ARG:HB2    | 9:K8:1089:LYS:HE2    | 1.56                     | 0.84              |
| 9:K8:635:ALA:CA      | 9:K8:655:GLN:NE2     | 2.25                     | 0.84              |
| 9:K8:1139:ILE:O      | 9:K8:1140:GLN:O      | 1.93                     | 0.84              |
| 10:C16:627:VAL:HG12  | 10:C16:628:GLY:N     | 1.91                     | 0.84              |
| 10:C16:1449:GLU:OE2  | 24:D8:1151:SER:HA    | 1.77                     | 0.84              |
| 10:C16:1466:ARG:HH12 | 11:A24:127:SER:CB    | 1.90                     | 0.84              |
| 11:A24:259:ILE:CG2   | 11:A24:276:LEU:HD22  | 2.07                     | 0.84              |
| 11:A24:440:LEU:HD13  | 11:A24:443:LEU:HD11  | 1.57                     | 0.84              |
| 10:C24:764:ILE:CD1   | 10:C24:781:VAL:HG21  | 2.08                     | 0.84              |
| 11:A40:694:GLU:OE1   | 24:D24:1398:ARG:HA   | 1.76                     | 0.84              |
| 13:V:833:ASN:OD1     | 13:V:834:PRO:HD2     | 1.78                     | 0.84              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:1593:TRP:CZ2   | 10:C:1603:PHE:HD2    | 1.96                     | 0.84              |
| 10:C8:1274:ALA:C    | 10:C8:1276:SER:H     | 1.84                     | 0.84              |
| 18:B:968:PHE:CE1    | 18:B:998:LEU:HD23    | 2.12                     | 0.84              |
| 18:B:1673:ARG:O     | 18:B:1676:VAL:CG2    | 2.22                     | 0.84              |
| 20:E8:432:ILE:CD1   | 24:D40:72:GLU:HG2    | 2.08                     | 0.84              |
| 20:E8:437:SER:C     | 20:E8:439:MET:H      | 1.85                     | 0.84              |
| 22:I8:289:LEU:HD22  | 22:I8:296:ARG:HH12   | 1.41                     | 0.84              |
| 10:C32:643:LEU:HD11 | 10:C32:679:ARG:HH12  | 1.41                     | 0.84              |
| 1:R16:1124:TRP:CZ2  | 4:T16:669:PRO:CG     | 2.61                     | 0.84              |
| 2:M16:399:THR:HG21  | 2:M16:480:ARG:HH21   | 1.40                     | 0.84              |
| 4:T:353:GLN:NE2     | 4:T:386:HIS:NE2      | 2.26                     | 0.84              |
| 7:Q16:199:GLY:O     | 7:Q16:219:GLY:HA3    | 1.78                     | 0.84              |
| 10:C16:593:ARG:NH1  | 10:C16:655:SER:HG    | 1.75                     | 0.84              |
| 14:W:515:CYS:CB     | 14:W:604:PRO:N       | 2.28                     | 0.84              |
| 14:W:631:TYR:CD1    | 15:J:554:LEU:HD11    | 2.11                     | 0.84              |
| 10:C:1439:ILE:HD12  | 10:C:1457:LEU:HD13   | 1.58                     | 0.84              |
| 10:C8:110:ARG:HH12  | 10:C8:118:LEU:HD11   | 1.41                     | 0.84              |
| 10:C8:586:PRO:HD2   | 10:C8:650:ARG:HH12   | 1.41                     | 0.84              |
| 11:A16:121:GLN:NE2  | 18:B:1559:ALA:HA     | 1.91                     | 0.84              |
| 19:4:103:GLN:NE2    | 19:4:411:LEU:HD13    | 1.92                     | 0.84              |
| 20:E:353:ILE:CD1    | 20:E:413:PHE:CA      | 2.53                     | 0.84              |
| 21:H24:366:MET:HE3  | 22:I24:332:MET:HE3   | 1.60                     | 0.84              |
| 21:H16:228:LEU:HD11 | 23:J16:593:VAL:HG22  | 1.58                     | 0.84              |
| 24:D40:854:GLU:OE1  | 24:D40:927:GLN:NE2   | 2.10                     | 0.84              |
| 10:C32:1703:ILE:HA  | 10:C32:1706:LEU:HD12 | 1.58                     | 0.84              |
| 1:R:1269:LEU:HD12   | 5:P:684:ARG:CD       | 2.08                     | 0.84              |
| 2:M:211:MET:HE3     | 3:N:280:ASN:C        | 2.02                     | 0.84              |
| 1:R8:1466:LYS:HD2   | 6:O8:160:LEU:CB      | 2.07                     | 0.84              |
| 2:M8:399:THR:CG2    | 2:M8:480:ARG:NH2     | 2.41                     | 0.84              |
| 2:M8:417:ARG:NH2    | 8:L8:415:PHE:CZ      | 2.45                     | 0.84              |
| 1:R16:1269:LEU:CD1  | 5:P16:684:ARG:CG     | 2.22                     | 0.84              |
| 2:M16:211:MET:HE3   | 3:N16:280:ASN:C      | 2.02                     | 0.84              |
| 9:K:1035:SER:HB3    | 9:K:1088:ASP:OD2     | 1.77                     | 0.84              |
| 10:C16:1121:ILE:CG2 | 10:C16:1133:ILE:HD13 | 2.07                     | 0.84              |
| 10:C24:854:LEU:HD23 | 10:C24:911:ILE:HD11  | 1.58                     | 0.84              |
| 11:A40:471:ASN:HD21 | 24:D32:1149:VAL:HB   | 1.41                     | 0.84              |
| 12:A:259:ILE:CG2    | 12:A:276:LEU:HD22    | 2.07                     | 0.84              |
| 10:C:65:PRO:HG2     | 10:C:96:ARG:HH22     | 1.42                     | 0.84              |
| 10:C8:764:ILE:CD1   | 10:C8:781:VAL:HG21   | 2.08                     | 0.84              |
| 10:C8:1290:HIS:CD2  | 10:C8:1334:MET:CE    | 2.61                     | 0.84              |
| 18:B8:1045:LYS:HZ1  | 18:B8:1100:LEU:CD2   | 1.89                     | 0.84              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 21:H:140:PRO:O      | 21:H:165:ALA:HB2    | 1.76                     | 0.84              |
| 23:J8:718:GLN:NE2   | 23:J8:737:TRP:CE3   | 2.46                     | 0.84              |
| 21:H24:322:LEU:HD22 | 22:I24:300:LEU:CD2  | 2.08                     | 0.84              |
| 10:C32:323:HIS:CE1  | 10:C32:327:ILE:CD1  | 2.61                     | 0.84              |
| 1:R8:1124:TRP:CZ2   | 4:T8:669:PRO:CG     | 2.61                     | 0.84              |
| 1:R8:1466:LYS:HD3   | 6:O8:160:LEU:HD22   | 1.59                     | 0.84              |
| 7:Q16:239:ARG:NH2   | 7:Q16:299:SER:O     | 2.10                     | 0.84              |
| 8:L8:175:ARG:NH1    | 12:A48:134:LYS:HD3  | 1.92                     | 0.84              |
| 9:K8:601:VAL:HG11   | 9:K8:673:SER:HB3    | 1.57                     | 0.84              |
| 11:A40:259:ILE:CG2  | 11:A40:276:LEU:HD22 | 2.07                     | 0.84              |
| 11:A40:273:ARG:HE   | 11:A40:479:LEU:HD23 | 1.42                     | 0.84              |
| 11:A40:440:LEU:HB3  | 11:A40:443:LEU:CD1  | 2.04                     | 0.84              |
| 13:V:910:GLU:HG3    | 14:W:787:MET:CE     | 2.07                     | 0.84              |
| 10:C:499:LEU:CD2    | 10:C:505:PHE:CE2    | 2.60                     | 0.84              |
| 10:C:1265:ARG:O     | 10:C:1268:ARG:CD    | 2.25                     | 0.84              |
| 11:A32:440:LEU:HB3  | 11:A32:443:LEU:CD1  | 2.04                     | 0.84              |
| 18:B:1439:LYS:HG2   | 18:B:1500:LEU:HD13  | 1.60                     | 0.84              |
| 18:B8:817:CYS:CB    | 18:B8:885:ARG:NH1   | 2.41                     | 0.84              |
| 19:48:103:GLN:NE2   | 19:48:411:LEU:HD13  | 1.92                     | 0.84              |
| 21:H:228:LEU:HD11   | 23:J32:593:VAL:HG22 | 1.59                     | 0.84              |
| 24:D24:853:MET:HB3  | 24:D24:885:TYR:CD2  | 2.13                     | 0.84              |
| 2:M:185:ARG:NH1     | 2:M:213:LEU:HD12    | 1.91                     | 0.83              |
| 3:N:1:MET:HB2       | 3:N:302:PRO:O       | 1.77                     | 0.83              |
| 2:M8:211:MET:HE3    | 3:N8:280:ASN:C      | 2.02                     | 0.83              |
| 5:P:16:PHE:CE2      | 5:P:461:HIS:CE1     | 2.66                     | 0.83              |
| 6:O:90:GLU:OE2      | 6:O:98:LYS:NZ       | 2.11                     | 0.83              |
| 5:P16:16:PHE:CE2    | 5:P16:461:HIS:CE1   | 2.65                     | 0.83              |
| 10:C16:798:VAL:HG11 | 10:C16:802:TRP:CZ2  | 2.13                     | 0.83              |
| 10:C24:499:LEU:CD2  | 10:C24:505:PHE:CE2  | 2.60                     | 0.83              |
| 10:C:847:ARG:CZ     | 10:C:911:ILE:H      | 1.89                     | 0.83              |
| 10:C:1424:GLN:NE2   | 10:C:1478:VAL:CG1   | 2.40                     | 0.83              |
| 22:I8:131:ARG:CG    | 23:J8:557:ARG:HH21  | 1.80                     | 0.83              |
| 24:D:1435:ARG:NH1   | 24:D:1448:TYR:HE2   | 1.30                     | 0.83              |
| 1:R8:1132:TYR:CE1   | 1:R8:1214:ILE:HD13  | 2.13                     | 0.83              |
| 3:N8:19:MET:CE      | 3:N8:23:GLY:O       | 2.25                     | 0.83              |
| 5:P:313:TRP:CZ2     | 5:P:345:MET:HE2     | 2.11                     | 0.83              |
| 5:P:377:LEU:HD12    | 14:W:23:PRO:CB      | 2.08                     | 0.83              |
| 9:K:1056:VAL:HG13   | 9:K:1059:ARG:HE     | 1.41                     | 0.83              |
| 10:C24:1708:ARG:NH2 | 21:H24:279:GLU:OE1  | 2.11                     | 0.83              |
| 14:W:645:HIS:CE1    | 14:W:649:LEU:HD11   | 2.11                     | 0.83              |
| 10:C:1389:ILE:HD12  | 10:C:1426:ARG:HH11  | 1.42                     | 0.83              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C8:798:VAL:HG11  | 10:C8:802:TRP:CZ2   | 2.13                     | 0.83              |
| 11:A16:440:LEU:HD13 | 11:A16:443:LEU:HD11 | 1.57                     | 0.83              |
| 18:B:1045:LYS:NZ    | 18:B:1100:LEU:CD2   | 2.41                     | 0.83              |
| 18:B8:1205:ILE:CD1  | 18:B8:1271:PHE:CD2  | 2.61                     | 0.83              |
| 23:J24:718:GLN:NE2  | 23:J24:737:TRP:CE3  | 2.45                     | 0.83              |
| 24:D:403:ARG:CB     | 24:D16:748:GLU:OE1  | 2.24                     | 0.83              |
| 24:D40:839:GLU:CG   | 24:D40:971:HIS:CD2  | 2.61                     | 0.83              |
| 10:C32:345:MET:HE3  | 10:C32:401:ILE:HD13 | 1.50                     | 0.83              |
| 10:C32:1265:ARG:O   | 10:C32:1268:ARG:CD  | 2.25                     | 0.83              |
| 1:R:1101:ARG:HD2    | 24:D:1459:LEU:O     | 1.78                     | 0.83              |
| 1:R:1335:ILE:CG1    | 10:C:1170:VAL:HG21  | 2.07                     | 0.83              |
| 1:R8:634:ARG:CD     | 4:T8:160:HIS:CE1    | 2.61                     | 0.83              |
| 1:R8:1449:TRP:CE3   | 2:M8:160:LEU:HD12   | 2.14                     | 0.83              |
| 2:M8:185:ARG:NH1    | 2:M8:213:LEU:HD12   | 1.91                     | 0.83              |
| 6:O:176:ASN:ND2     | 6:O:179:LYS:HE3     | 1.93                     | 0.83              |
| 6:O8:90:GLU:OE2     | 6:O8:98:LYS:NZ      | 2.11                     | 0.83              |
| 10:C16:249:THR:C    | 10:C16:251:GLY:N    | 2.37                     | 0.83              |
| 10:C24:798:VAL:HG11 | 10:C24:802:TRP:CZ2  | 2.13                     | 0.83              |
| 10:C:843:MET:HE3    | 10:C:911:ILE:HG12   | 1.61                     | 0.83              |
| 10:C:1010:ALA:CA    | 10:C:1192:ARG:HH21  | 1.92                     | 0.83              |
| 10:C8:1424:GLN:NE2  | 10:C8:1478:VAL:CG1  | 2.40                     | 0.83              |
| 18:B:817:CYS:CB     | 18:B:885:ARG:NH1    | 2.41                     | 0.83              |
| 18:B8:1618:HIS:HE1  | 18:B8:1622:ILE:HD11 | 1.39                     | 0.83              |
| 20:E8:434:TRP:NE1   | 24:D40:72:GLU:CG    | 2.17                     | 0.83              |
| 20:E8:447:ILE:CG2   | 20:E8:451:ILE:CG2   | 2.57                     | 0.83              |
| 23:J16:718:GLN:NE2  | 23:J16:737:TRP:CE3  | 2.46                     | 0.83              |
| 10:C32:643:LEU:HD21 | 10:C32:675:ASP:CG   | 2.03                     | 0.83              |
| 10:C32:1274:ALA:C   | 10:C32:1276:SER:H   | 1.85                     | 0.83              |
| 1:R16:1132:TYR:CE1  | 1:R16:1214:ILE:HD13 | 2.13                     | 0.83              |
| 7:Q8:239:ARG:NH2    | 7:Q8:299:SER:O      | 2.10                     | 0.83              |
| 6:O16:90:GLU:OE2    | 6:O16:98:LYS:NZ     | 2.11                     | 0.83              |
| 6:O16:176:ASN:ND2   | 6:O16:179:LYS:HE3   | 1.93                     | 0.83              |
| 9:K8:1137:LEU:HD23  | 9:K8:1173:ASN:HD22  | 1.42                     | 0.83              |
| 10:C16:323:HIS:CE1  | 10:C16:327:ILE:CD1  | 2.61                     | 0.83              |
| 10:C16:764:ILE:CD1  | 10:C16:781:VAL:HG21 | 2.08                     | 0.83              |
| 10:C24:1593:TRP:CZ2 | 10:C24:1603:PHE:HD2 | 1.96                     | 0.83              |
| 10:C:764:ILE:CD1    | 10:C:781:VAL:HG21   | 2.08                     | 0.83              |
| 10:C:1265:ARG:O     | 10:C:1268:ARG:HG3   | 1.75                     | 0.83              |
| 10:C8:1593:TRP:CZ2  | 10:C8:1603:PHE:HD2  | 1.96                     | 0.83              |
| 11:A16:388:VAL:N    | 11:A16:459:ARG:HH12 | 1.73                     | 0.83              |
| 11:A32:56:ALA:C     | 11:A32:58:SER:H     | 1.86                     | 0.83              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:440:LEU:CB    | 11:A32:443:LEU:HD11  | 2.07                     | 0.83              |
| 18:B:1156:GLN:O      | 18:B:1382:LYS:NZ     | 2.10                     | 0.83              |
| 19:4:4:PHE:CE2       | 19:4:378:TYR:CD1     | 2.65                     | 0.83              |
| 20:E:437:SER:C       | 20:E:439:MET:H       | 1.85                     | 0.83              |
| 19:48:100:ILE:HD11   | 19:48:274:PHE:HE1    | 1.41                     | 0.83              |
| 10:C32:572:ILE:CD1   | 10:C32:606:MET:HE1   | 2.08                     | 0.83              |
| 10:C32:764:ILE:CD1   | 10:C32:781:VAL:HG21  | 2.08                     | 0.83              |
| 1:R:1191:LYS:HB2     | 24:D:1453:GLU:CG     | 2.08                     | 0.83              |
| 1:R:1425:PRO:CA      | 6:O:165:LYS:HZ3      | 1.85                     | 0.83              |
| 3:N:19:MET:CE        | 3:N:23:GLY:O         | 2.25                     | 0.83              |
| 2:M8:628:LEU:CD1     | 3:N8:223:GLY:C       | 2.51                     | 0.83              |
| 1:R16:634:ARG:CD     | 4:T16:160:HIS:CE1    | 2.61                     | 0.83              |
| 5:P:607:PHE:CZ       | 5:P:611:LEU:CD1      | 2.62                     | 0.83              |
| 7:Q8:297:VAL:HG12    | 7:Q8:301:ARG:HB2     | 1.58                     | 0.83              |
| 8:L8:976:LEU:HD22    | 9:K8:1004:ARG:HD3    | 0.83                     | 0.83              |
| 9:K:1180:TRP:CZ2     | 9:K:1206:LEU:HD12    | 2.12                     | 0.83              |
| 10:C16:499:LEU:CD2   | 10:C16:505:PHE:CE2   | 2.60                     | 0.83              |
| 10:C16:1126:ASP:OD2  | 24:D8:1069:GLY:CA    | 2.25                     | 0.83              |
| 10:C24:643:LEU:HD21  | 10:C24:675:ASP:CG    | 2.03                     | 0.83              |
| 10:C24:1290:HIS:CD2  | 10:C24:1334:MET:HE2  | 2.14                     | 0.83              |
| 11:A40:56:ALA:C      | 11:A40:58:SER:H      | 1.86                     | 0.83              |
| 12:A:288:HIS:HB2     | 12:A:354:ARG:NH1     | 1.92                     | 0.83              |
| 10:C:572:ILE:CD1     | 10:C:606:MET:HE1     | 2.08                     | 0.83              |
| 18:B8:682:TYR:O      | 18:B8:684:ILE:N      | 2.10                     | 0.83              |
| 20:E8:202:ASP:C      | 20:E8:204:SER:H      | 1.86                     | 0.83              |
| 20:E8:354:ASP:OD1    | 20:E8:355:PRO:HD2    | 1.77                     | 0.83              |
| 10:C32:1389:ILE:HD12 | 10:C32:1426:ARG:HH11 | 1.42                     | 0.83              |
| 1:R16:1269:LEU:HD12  | 5:P16:684:ARG:NE     | 1.91                     | 0.83              |
| 7:Q8:241:HIS:CD2     | 7:Q8:258:ARG:NE      | 2.47                     | 0.83              |
| 8:L8:270:LEU:HD21    | 12:A48:155:SER:CB    | 2.09                     | 0.83              |
| 10:C16:1703:ILE:HA   | 10:C16:1706:LEU:HD12 | 1.59                     | 0.83              |
| 10:C24:627:VAL:HG12  | 10:C24:628:GLY:N     | 1.91                     | 0.83              |
| 10:C24:847:ARG:CZ    | 10:C24:911:ILE:H     | 1.89                     | 0.83              |
| 10:C:345:MET:HE1     | 10:C:401:ILE:HD13    | 1.40                     | 0.83              |
| 10:C:798:VAL:HG11    | 10:C:802:TRP:CZ2     | 2.13                     | 0.83              |
| 10:C:1274:ALA:C      | 10:C:1276:SER:H      | 1.84                     | 0.83              |
| 10:C8:572:ILE:CD1    | 10:C8:606:MET:HE1    | 2.08                     | 0.83              |
| 11:A16:36:ASN:ND2    | 22:I:293:LYS:HE2     | 1.92                     | 0.83              |
| 11:A32:288:HIS:HB2   | 11:A32:354:ARG:NH1   | 1.92                     | 0.83              |
| 11:A32:676:TYR:HE2   | 24:D32:1396:PRO:HD2  | 1.33                     | 0.83              |
| 18:B:1291:LEU:HD11   | 18:B:1332:VAL:HG21   | 1.61                     | 0.83              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 20:E:354:ASP:OD1     | 20:E:355:PRO:HD2     | 1.77                     | 0.83              |
| 5:P:109:ILE:HG12     | 14:W:18:PRO:CD       | 2.08                     | 0.83              |
| 7:Q:199:GLY:O        | 7:Q:219:GLY:HA3      | 1.77                     | 0.83              |
| 9:K:916:LYS:HG2      | 9:K:919:MET:HE2      | 0.83                     | 0.83              |
| 10:C24:450:PRO:HB3   | 10:C24:485:THR:O     | 1.77                     | 0.83              |
| 13:V:839:LYS:NZ      | 15:J:652:GLU:HG2     | 1.93                     | 0.83              |
| 10:C:110:ARG:HH12    | 10:C:118:LEU:HD11    | 1.41                     | 0.83              |
| 11:A16:362:ARG:HD2   | 11:A16:366:ARG:HH22  | 1.04                     | 0.83              |
| 11:A32:362:ARG:HD2   | 11:A32:366:ARG:HH22  | 1.04                     | 0.83              |
| 18:B:457:SER:HA      | 18:B:548:ARG:HH11    | 1.40                     | 0.83              |
| 18:B:1575:GLN:NE2    | 24:D16:1403:LEU:CG   | 2.41                     | 0.83              |
| 20:E:447:ILE:CG2     | 20:E:451:ILE:CG2     | 2.57                     | 0.83              |
| 19:48:189:LEU:CD1    | 19:48:203:LEU:CD2    | 2.50                     | 0.83              |
| 10:C32:1439:ILE:HD12 | 10:C32:1457:LEU:HD13 | 1.58                     | 0.83              |
| 2:M:628:LEU:CD1      | 3:N:223:GLY:HA3      | 2.09                     | 0.83              |
| 2:M8:345:ASP:C       | 2:M8:347:LYS:N       | 2.31                     | 0.83              |
| 2:M8:622:ARG:NH2     | 2:M8:624:ASP:OD2     | 2.10                     | 0.83              |
| 1:R16:1223:PHE:CE1   | 5:P16:676:GLN:CD     | 2.57                     | 0.83              |
| 1:R16:1449:TRP:CE3   | 2:M16:160:LEU:HD12   | 2.14                     | 0.83              |
| 4:T8:353:GLN:NE2     | 4:T8:386:HIS:NE2     | 2.26                     | 0.83              |
| 4:T16:353:GLN:NE2    | 4:T16:386:HIS:NE2    | 2.26                     | 0.83              |
| 5:P8:607:PHE:CZ      | 5:P8:611:LEU:CD1     | 2.62                     | 0.83              |
| 8:L:1089:MET:HE3     | 9:K:1000:SER:CB      | 2.09                     | 0.83              |
| 9:K:847:LEU:HD21     | 9:K:910:SER:HG       | 1.39                     | 0.83              |
| 10:C24:386:ASN:CG    | 10:C24:449:GLU:OE1   | 2.22                     | 0.83              |
| 10:C24:1708:ARG:NH1  | 21:H24:279:GLU:CG    | 2.42                     | 0.83              |
| 11:A40:15:HIS:CE1    | 22:I16:165:GLY:O     | 2.32                     | 0.83              |
| 10:C8:186:LEU:HD22   | 10:C8:206:ARG:HG2    | 1.59                     | 0.83              |
| 11:A16:273:ARG:HE    | 11:A16:479:LEU:HD23  | 1.42                     | 0.83              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:HG21   | 1.59                     | 0.83              |
| 19:48:63:GLY:O       | 19:48:65:LYS:N       | 2.12                     | 0.83              |
| 24:D40:839:GLU:CD    | 24:D40:971:HIS:CG    | 2.57                     | 0.83              |
| 10:C32:450:PRO:HB3   | 10:C32:485:THR:O     | 1.77                     | 0.83              |
| 10:C32:798:VAL:HG11  | 10:C32:802:TRP:CZ2   | 2.13                     | 0.83              |
| 2:M16:351:ALA:CB     | 8:L16:219:ILE:HG21   | 2.04                     | 0.83              |
| 5:P:401:ARG:CD       | 5:P:414:VAL:CG1      | 2.57                     | 0.83              |
| 7:Q:239:ARG:NH2      | 7:Q:299:SER:O        | 2.10                     | 0.83              |
| 7:Q:241:HIS:CD2      | 7:Q:258:ARG:NE       | 2.47                     | 0.83              |
| 7:Q8:199:GLY:O       | 7:Q8:219:GLY:HA3     | 1.78                     | 0.83              |
| 8:L:1069:LEU:CD1     | 9:K:1086:VAL:HG11    | 2.07                     | 0.83              |
| 10:C16:643:LEU:HD21  | 10:C16:675:ASP:CG    | 2.03                     | 0.83              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C16:847:ARG:CZ   | 10:C16:911:ILE:H     | 1.88                     | 0.83              |
| 10:C16:1290:HIS:CD2 | 10:C16:1334:MET:HE2  | 2.14                     | 0.83              |
| 10:C16:1453:ARG:CZ  | 24:D8:1150:GLY:HA3   | 2.09                     | 0.83              |
| 11:A24:56:ALA:C     | 11:A24:58:SER:H      | 1.86                     | 0.83              |
| 11:A24:440:LEU:HB3  | 11:A24:443:LEU:CD1   | 2.04                     | 0.83              |
| 11:A40:440:LEU:CB   | 11:A40:443:LEU:HD11  | 2.07                     | 0.83              |
| 13:V:814:MET:HE3    | 13:V:824:TRP:CZ2     | 2.13                     | 0.83              |
| 14:W:701:LEU:HD11   | 15:J:624:ALA:HB1     | 1.56                     | 0.83              |
| 10:C:323:HIS:CE1    | 10:C:327:ILE:CD1     | 2.61                     | 0.83              |
| 10:C8:1265:ARG:O    | 10:C8:1268:ARG:CD    | 2.25                     | 0.83              |
| 10:C8:1290:HIS:CD2  | 10:C8:1334:MET:HE2   | 2.14                     | 0.83              |
| 18:B:682:TYR:O      | 18:B:684:ILE:N       | 2.10                     | 0.83              |
| 18:B:1175:ALA:HB1   | 18:B:1272:TRP:CD1    | 2.14                     | 0.83              |
| 18:B8:1175:ALA:HB1  | 18:B8:1272:TRP:CD1   | 2.14                     | 0.83              |
| 19:48:4:PHE:CE2     | 19:48:378:TYR:CD1    | 2.65                     | 0.83              |
| 21:H:322:LEU:HD22   | 22:I:300:LEU:CD2     | 2.08                     | 0.83              |
| 10:C32:1430:ARG:HG3 | 10:C32:1482:MET:HE2  | 1.61                     | 0.83              |
| 6:O:119:ARG:NH2     | 6:O:182:GLU:CG       | 2.40                     | 0.83              |
| 7:Q8:149:VAL:HG23   | 7:Q8:187:TRP:CZ2     | 2.14                     | 0.83              |
| 7:Q16:241:HIS:CD2   | 7:Q16:258:ARG:NE     | 2.46                     | 0.83              |
| 9:K:1039:ASP:OD2    | 9:K:1096:LYS:NZ      | 2.11                     | 0.83              |
| 9:K8:919:MET:SD     | 9:K8:923:ILE:HD11    | 2.19                     | 0.83              |
| 11:A24:440:LEU:CB   | 11:A24:443:LEU:HD11  | 2.07                     | 0.83              |
| 10:C24:417:LEU:HB3  | 10:C24:472:ASN:ND2   | 1.94                     | 0.83              |
| 10:C24:1703:ILE:HA  | 10:C24:1706:LEU:HD12 | 1.58                     | 0.83              |
| 10:C:52:SER:OG      | 24:D:1017:GLN:CG     | 2.23                     | 0.83              |
| 11:A16:440:LEU:CB   | 11:A16:443:LEU:HD11  | 2.07                     | 0.83              |
| 22:I24:290:ASP:OD1  | 22:I24:293:LYS:HE3   | 1.79                     | 0.83              |
| 21:H16:288:THR:OG1  | 23:J16:650:GLN:NE2   | 2.12                     | 0.83              |
| 21:H16:366:MET:HE3  | 22:I16:332:MET:HE3   | 1.60                     | 0.83              |
| 10:C32:286:ILE:CG2  | 10:C32:292:PHE:CE1   | 2.62                     | 0.83              |
| 9:K8:1180:TRP:CZ2   | 9:K8:1206:LEU:HD12   | 2.13                     | 0.82              |
| 10:C16:572:ILE:CD1  | 10:C16:606:MET:HE1   | 2.08                     | 0.82              |
| 10:C16:1593:TRP:CZ2 | 10:C16:1603:PHE:HD2  | 1.96                     | 0.82              |
| 11:A24:15:HIS:CE1   | 22:I8:165:GLY:O      | 2.32                     | 0.82              |
| 10:C24:847:ARG:NE   | 10:C24:903:ASN:OD1   | 2.12                     | 0.82              |
| 12:A:273:ARG:HE     | 12:A:479:LEU:HD23    | 1.42                     | 0.82              |
| 10:C8:286:ILE:CG2   | 10:C8:292:PHE:CE1    | 2.62                     | 0.82              |
| 10:C8:323:HIS:CE1   | 10:C8:327:ILE:CD1    | 2.61                     | 0.82              |
| 11:A16:288:HIS:HB2  | 11:A16:354:ARG:NH1   | 1.92                     | 0.82              |
| 11:A16:696:ILE:CD1  | 11:A16:728:ILE:HD12  | 2.09                     | 0.82              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A32:15:HIS:CE1   | 22:I24:165:GLY:O     | 2.31                     | 0.82              |
| 11:A32:696:ILE:CD1  | 11:A32:728:ILE:HD12  | 2.09                     | 0.82              |
| 18:B:1155:ILE:O     | 18:B:1159:SER:OG     | 1.95                     | 0.82              |
| 10:C32:843:MET:HE3  | 10:C32:911:ILE:HG12  | 1.61                     | 0.82              |
| 10:C32:1290:HIS:CD2 | 10:C32:1334:MET:HE2  | 2.14                     | 0.82              |
| 12:A48:696:ILE:CD1  | 12:A48:728:ILE:HD12  | 2.09                     | 0.82              |
| 3:N8:1:MET:HB2      | 3:N8:302:PRO:O       | 1.77                     | 0.82              |
| 2:M16:414:GLY:HA2   | 8:L16:401:LYS:HZ3    | 1.42                     | 0.82              |
| 5:P:322:CYS:CB      | 13:V:767:GLU:OE2     | 2.28                     | 0.82              |
| 9:K:1137:LEU:HD23   | 9:K:1173:ASN:HD22    | 1.42                     | 0.82              |
| 9:K:1230:LEU:HD23   | 9:K:1244:VAL:CG2     | 2.09                     | 0.82              |
| 9:K8:1230:LEU:HD23  | 9:K8:1244:VAL:CG2    | 2.09                     | 0.82              |
| 11:A40:390:ALA:HB1  | 24:D32:1099:ARG:HB2  | 1.61                     | 0.82              |
| 11:A40:474:LEU:HD13 | 24:D32:1099:ARG:HH12 | 1.40                     | 0.82              |
| 10:C:1285:VAL:HA    | 10:C:1735:TYR:HE2    | 1.41                     | 0.82              |
| 10:C8:1430:ARG:HG3  | 10:C8:1482:MET:HE2   | 1.60                     | 0.82              |
| 18:B8:1156:GLN:O    | 18:B8:1382:LYS:NZ    | 2.10                     | 0.82              |
| 19:4:63:GLY:O       | 19:4:65:LYS:N        | 2.12                     | 0.82              |
| 20:E:352:PHE:HE1    | 20:E:451:ILE:HD13    | 1.03                     | 0.82              |
| 21:H24:288:THR:OG1  | 23:J24:650:GLN:NE2   | 2.12                     | 0.82              |
| 10:C32:1593:TRP:CZ2 | 10:C32:1603:PHE:HD2  | 1.96                     | 0.82              |
| 2:M16:540:TYR:HE1   | 2:M16:555:LEU:CD2    | 1.77                     | 0.82              |
| 5:P:325:PHE:CZ      | 13:V:771:GLN:NE2     | 2.46                     | 0.82              |
| 5:P8:16:PHE:CE2     | 5:P8:461:HIS:CE1     | 2.66                     | 0.82              |
| 9:K8:638:TRP:CZ3    | 9:K8:754:ARG:HD2     | 2.14                     | 0.82              |
| 10:C16:286:ILE:CG2  | 10:C16:292:PHE:CE1   | 2.62                     | 0.82              |
| 10:C16:1265:ARG:O   | 10:C16:1268:ARG:HG3  | 1.75                     | 0.82              |
| 10:C16:1688:ARG:HG3 | 23:J32:735:LYS:HE3   | 1.48                     | 0.82              |
| 10:C:110:ARG:HH11   | 10:C:118:LEU:HD11    | 1.00                     | 0.82              |
| 10:C8:1285:VAL:HG23 | 10:C8:1738:MET:HE2   | 1.46                     | 0.82              |
| 11:A16:703:ALA:O    | 24:D16:1398:ARG:CZ   | 2.27                     | 0.82              |
| 18:B:779:LYS:HE2    | 18:B:847:GLN:HE21    | 1.38                     | 0.82              |
| 21:H:288:THR:OG1    | 23:J32:650:GLN:NE2   | 2.12                     | 0.82              |
| 10:C32:453:LEU:CD2  | 10:C32:459:LEU:HD11  | 2.08                     | 0.82              |
| 1:R:1449:TRP:CE3    | 2:M:160:LEU:HD12     | 2.14                     | 0.82              |
| 2:M:628:LEU:CD1     | 3:N:223:GLY:C        | 2.51                     | 0.82              |
| 4:T16:671:ILE:HD11  | 5:P16:698:GLY:HA3    | 1.61                     | 0.82              |
| 7:Q16:221:TRP:CZ3   | 7:Q16:222:PHE:HE2    | 1.97                     | 0.82              |
| 9:K8:1053:MET:O     | 9:K8:1054:THR:C      | 2.12                     | 0.82              |
| 10:C24:323:HIS:CE1  | 10:C24:327:ILE:CD1   | 2.61                     | 0.82              |
| 14:W:586:ILE:CD1    | 15:J:572:ASP:CB      | 2.49                     | 0.82              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C8:450:PRO:HB3   | 10:C8:485:THR:O      | 1.77                     | 0.82              |
| 18:B:496:LEU:CD2    | 18:B:540:ILE:HD12    | 2.10                     | 0.82              |
| 18:B:1205:ILE:CD1   | 18:B:1271:PHE:CD2    | 2.61                     | 0.82              |
| 19:48:340:PRO:HD3   | 24:D8:140:ALA:HB1    | 1.61                     | 0.82              |
| 21:H8:322:LEU:HD22  | 22:I8:300:LEU:CD2    | 2.08                     | 0.82              |
| 24:D:1:MET:CB       | 24:D:882:GLU:OE2     | 2.27                     | 0.82              |
| 24:D:403:ARG:NH2    | 24:D:409:LEU:HD11    | 1.93                     | 0.82              |
| 1:R:1132:TYR:CE1    | 1:R:1214:ILE:HD13    | 2.13                     | 0.82              |
| 2:M:399:THR:HG21    | 2:M:480:ARG:HH21     | 1.40                     | 0.82              |
| 2:M16:627:TYR:CE2   | 3:N16:166:ALA:O      | 2.32                     | 0.82              |
| 9:K8:853:ALA:CB     | 9:K8:856:ILE:HD12    | 2.10                     | 0.82              |
| 10:C16:389:LEU:HD21 | 10:C16:447:PHE:HE1   | 1.41                     | 0.82              |
| 18:B:1161:LEU:HD23  | 18:B:1164:GLU:OE2    | 1.79                     | 0.82              |
| 18:B8:65:LEU:HD23   | 18:B8:79:ILE:HD12    | 1.62                     | 0.82              |
| 18:B8:496:LEU:CD2   | 18:B8:540:ILE:HD12   | 2.10                     | 0.82              |
| 19:48:153:ARG:HH21  | 20:E8:467:ILE:HD11   | 1.39                     | 0.82              |
| 23:J32:718:GLN:NE2  | 23:J32:737:TRP:CE3   | 2.45                     | 0.82              |
| 21:H8:366:MET:HE3   | 22:I8:332:MET:HE3    | 1.60                     | 0.82              |
| 22:I24:199:PHE:CG   | 23:J24:620:MET:SD    | 2.73                     | 0.82              |
| 10:C32:1010:ALA:CA  | 10:C32:1192:ARG:HH21 | 1.92                     | 0.82              |
| 1:R:1139:ARG:HB2    | 1:R:1157:ARG:CZ      | 2.08                     | 0.82              |
| 2:M16:593:HIS:CD2   | 3:N16:224:LEU:HD22   | 2.15                     | 0.82              |
| 2:M16:847:PHE:HB3   | 4:T16:656:TRP:CZ3    | 2.14                     | 0.82              |
| 5:P:251:LYS:HE3     | 14:W:765:LYS:CE      | 2.09                     | 0.82              |
| 7:Q:149:VAL:HG23    | 7:Q:187:TRP:CZ2      | 2.14                     | 0.82              |
| 8:L8:598:LEU:HD21   | 8:L8:627:ARG:NH2     | 1.93                     | 0.82              |
| 10:C16:1547:LYS:CE  | 24:D8:1405:GLY:H     | 1.92                     | 0.82              |
| 11:A24:645:GLU:OE1  | 24:D16:867:ASP:OD1   | 1.95                     | 0.82              |
| 11:A40:36:ASN:ND2   | 22:I16:293:LYS:HE2   | 1.92                     | 0.82              |
| 11:A40:440:LEU:HD13 | 11:A40:443:LEU:HD11  | 1.57                     | 0.82              |
| 14:W:711:ARG:CD     | 10:C8:1609:ASP:CG    | 2.53                     | 0.82              |
| 10:C8:847:ARG:NE    | 10:C8:903:ASN:OD1    | 2.12                     | 0.82              |
| 18:B8:1529:GLU:OE2  | 24:D32:1415:LEU:CD2  | 2.28                     | 0.82              |
| 19:4:332:PRO:HD3    | 20:E:294:VAL:HG13    | 1.61                     | 0.82              |
| 21:H:366:MET:HE3    | 22:I:332:MET:HE3     | 1.60                     | 0.82              |
| 21:H16:322:LEU:HD22 | 22:I16:300:LEU:CD2   | 2.08                     | 0.82              |
| 10:C32:847:ARG:NE   | 10:C32:903:ASN:OD1   | 2.12                     | 0.82              |
| 2:M:762:LEU:HB2     | 2:M:813:ASN:HD21     | 0.90                     | 0.82              |
| 2:M:847:PHE:HB3     | 4:T:656:TRP:CZ3      | 2.14                     | 0.82              |
| 2:M16:628:LEU:CD1   | 3:N16:223:GLY:HA3    | 2.09                     | 0.82              |
| 2:M16:672:TYR:HB3   | 2:M16:680:LYS:CD     | 1.93                     | 0.82              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P:42:SER:HA        | 6:O:287:GLU:OE2      | 1.79                     | 0.82              |
| 5:P:401:ARG:HH21     | 5:P:404:ILE:HG21     | 1.43                     | 0.82              |
| 9:K8:847:LEU:HD21    | 9:K8:910:SER:CB      | 2.09                     | 0.82              |
| 11:A24:36:ASN:ND2    | 22:I8:293:LYS:HE2    | 1.93                     | 0.82              |
| 12:A:696:ILE:CD1     | 12:A:728:ILE:HD12    | 2.09                     | 0.82              |
| 14:W:711:ARG:CZ      | 10:C8:1606:GLY:HA2   | 2.09                     | 0.82              |
| 10:C:286:ILE:CG2     | 10:C:292:PHE:CE1     | 2.62                     | 0.82              |
| 10:C:982:LEU:HD13    | 10:C:1025:LEU:HD21   | 1.61                     | 0.82              |
| 18:B:1205:ILE:HD11   | 18:B:1271:PHE:HD2    | 1.43                     | 0.82              |
| 19:48:183:ARG:NH2    | 19:48:242:VAL:O      | 2.13                     | 0.82              |
| 1:R:1165:MET:CE      | 1:R:1220:GLN:HG2     | 2.09                     | 0.82              |
| 2:M:210:GLN:CD       | 10:C:529:GLN:HE22    | 1.88                     | 0.82              |
| 2:M8:552:PHE:HZ      | 2:M8:559:PHE:HE2     | 1.28                     | 0.82              |
| 2:M8:628:LEU:CD1     | 3:N8:223:GLY:HA3     | 2.09                     | 0.82              |
| 2:M16:401:ARG:HH22   | 8:L16:381:GLU:CB     | 1.87                     | 0.82              |
| 5:P:510:ILE:CD1      | 7:Q:183:ARG:HH12     | 1.93                     | 0.82              |
| 7:Q8:98:MET:HE2      | 7:Q8:110:VAL:CG1     | 2.10                     | 0.82              |
| 9:K8:1039:ASP:OD2    | 9:K8:1096:LYS:NZ     | 2.11                     | 0.82              |
| 10:C16:1010:ALA:CA   | 10:C16:1192:ARG:HH21 | 1.92                     | 0.82              |
| 10:C24:390:HIS:HB3   | 10:C24:452:LEU:HG    | 0.83                     | 0.82              |
| 10:C24:1285:VAL:HG21 | 10:C24:1738:MET:HE3  | 1.61                     | 0.82              |
| 13:V:783:TRP:CH2     | 14:W:671:GLU:HA      | 2.13                     | 0.82              |
| 10:C:1430:ARG:HG3    | 10:C:1482:MET:HE2    | 1.61                     | 0.82              |
| 18:B8:1291:LEU:HD11  | 18:B8:1332:VAL:HG21  | 1.60                     | 0.82              |
| 20:E:202:ASP:C       | 20:E:204:SER:H       | 1.86                     | 0.82              |
| 21:H8:288:THR:OG1    | 23:J8:650:GLN:NE2    | 2.12                     | 0.82              |
| 5:P:109:ILE:HG23     | 14:W:18:PRO:HG2      | 1.59                     | 0.82              |
| 5:P16:506:ASN:ND2    | 7:Q16:153:GLU:OE1    | 2.13                     | 0.82              |
| 5:P16:603:LYS:O      | 5:P16:607:PHE:CD1    | 2.33                     | 0.82              |
| 9:K:638:TRP:CZ3      | 9:K:754:ARG:HD2      | 2.14                     | 0.82              |
| 10:C16:1271:PHE:HZ   | 10:C16:1284:ASP:CG   | 1.75                     | 0.82              |
| 11:A24:54:ASN:HB3    | 11:A24:59:GLN:HE22   | 1.45                     | 0.82              |
| 10:C8:843:MET:HE3    | 10:C8:911:ILE:HG12   | 1.60                     | 0.82              |
| 10:C8:1010:ALA:CA    | 10:C8:1192:ARG:HH21  | 1.92                     | 0.82              |
| 11:A16:56:ALA:C      | 11:A16:58:SER:H      | 1.86                     | 0.82              |
| 11:A16:90:PHE:CA     | 18:B:1800:ARG:NH2    | 2.42                     | 0.82              |
| 18:B8:13:TRP:O       | 18:B8:107:ARG:NH2    | 2.12                     | 0.82              |
| 18:B8:671:MET:CE     | 18:B8:736:ALA:HB2    | 2.09                     | 0.82              |
| 18:B8:1161:LEU:HD23  | 18:B8:1164:GLU:OE2   | 1.79                     | 0.82              |
| 21:H8:247:GLU:OE2    | 22:I8:181:LEU:HD23   | 1.80                     | 0.82              |
| 24:D:1099:ARG:NE     | 24:D:1149:VAL:HG21   | 1.93                     | 0.82              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C32:407:LYS:CE   | 10:C32:465:PHE:HE2  | 1.93                     | 0.82              |
| 3:N:19:MET:CE       | 3:N:23:GLY:C        | 2.50                     | 0.82              |
| 1:R8:1132:TYR:CE1   | 1:R8:1214:ILE:CD1   | 2.63                     | 0.82              |
| 2:M8:627:TYR:CE2    | 3:N8:162:THR:HB     | 2.14                     | 0.82              |
| 1:R16:1132:TYR:CE1  | 1:R16:1214:ILE:CD1  | 2.63                     | 0.82              |
| 2:M16:451:PHE:O     | 8:L16:295:HIS:HD2   | 1.62                     | 0.82              |
| 2:M16:544:LEU:HG    | 2:M16:586:ALA:HB1   | 1.61                     | 0.82              |
| 2:M16:816:ARG:HH12  | 2:M16:849:LEU:C     | 1.88                     | 0.82              |
| 5:P:152:ILE:HG21    | 14:W:762:GLN:HE22   | 1.43                     | 0.82              |
| 7:Q:297:VAL:HG12    | 7:Q:301:ARG:HB2     | 1.58                     | 0.82              |
| 7:Q8:221:TRP:CZ3    | 7:Q8:222:PHE:HE2    | 1.97                     | 0.82              |
| 10:C16:565:ARG:CD   | 10:C16:568:TRP:HE3  | 1.92                     | 0.82              |
| 10:C24:286:ILE:CG2  | 10:C24:292:PHE:CE1  | 2.62                     | 0.82              |
| 10:C24:578:LEU:HB3  | 10:C24:584:ILE:HD13 | 1.62                     | 0.82              |
| 10:C24:1691:GLU:CD  | 23:J24:735:LYS:HA   | 2.04                     | 0.82              |
| 10:C:249:THR:C      | 10:C:251:GLY:N      | 2.36                     | 0.82              |
| 18:B8:86:LYS:HE2    | 18:B8:123:LEU:CD1   | 2.10                     | 0.82              |
| 21:H16:247:GLU:OE2  | 22:I16:181:LEU:HD23 | 1.80                     | 0.82              |
| 22:I16:146:SER:OG   | 23:J16:574:ARG:NH1  | 2.13                     | 0.82              |
| 24:D40:873:ARG:CZ   | 24:D40:884:ASP:HB3  | 2.10                     | 0.82              |
| 10:C32:186:LEU:HD22 | 10:C32:206:ARG:HG2  | 1.58                     | 0.82              |
| 10:C32:417:LEU:HB3  | 10:C32:472:ASN:ND2  | 1.94                     | 0.82              |
| 10:C32:1271:PHE:CZ  | 10:C32:1284:ASP:OD1 | 2.29                     | 0.82              |
| 2:M:593:HIS:CD2     | 3:N:224:LEU:HD22    | 2.15                     | 0.81              |
| 2:M:816:ARG:HH12    | 2:M:849:LEU:C       | 1.88                     | 0.81              |
| 1:R8:1125:ARG:NH2   | 2:M8:834:ASP:OD2    | 2.13                     | 0.81              |
| 2:M16:417:ARG:HD2   | 8:L16:298:PHE:CD2   | 2.11                     | 0.81              |
| 8:L8:270:LEU:HD23   | 12:A48:155:SER:CB   | 2.00                     | 0.81              |
| 10:C16:389:LEU:CD2  | 10:C16:447:PHE:CE1  | 2.60                     | 0.81              |
| 10:C16:847:ARG:NE   | 10:C16:903:ASN:OD1  | 2.12                     | 0.81              |
| 11:A24:707:LEU:CD2  | 11:A24:767:ARG:NH2  | 2.43                     | 0.81              |
| 11:A40:54:ASN:HB3   | 11:A40:59:GLN:HE22  | 1.45                     | 0.81              |
| 11:A40:696:ILE:CD1  | 11:A40:728:ILE:HD12 | 2.09                     | 0.81              |
| 11:A16:15:HIS:CE1   | 22:I:165:GLY:O      | 2.32                     | 0.81              |
| 11:A16:54:ASN:HB3   | 11:A16:59:GLN:HE22  | 1.45                     | 0.81              |
| 11:A16:270:VAL:HG12 | 11:A16:274:MET:HB3  | 1.62                     | 0.81              |
| 11:A16:326:TYR:HD1  | 17:F8:77:TYR:CB     | 1.83                     | 0.81              |
| 11:A32:273:ARG:HE   | 11:A32:479:LEU:HD23 | 1.42                     | 0.81              |
| 19:4:250:ILE:CD1    | 20:E:165:ARG:HH21   | 1.93                     | 0.81              |
| 10:C32:452:LEU:HD23 | 10:C32:452:LEU:H    | 1.44                     | 0.81              |
| 1:R:1125:ARG:NH2    | 2:M:834:ASP:OD2     | 2.13                     | 0.81              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M8:225:ASP:HB3    | 2:M8:606:GLN:HE21   | 1.45                     | 0.81              |
| 2:M16:225:ASP:HB3   | 2:M16:606:GLN:HE21  | 1.45                     | 0.81              |
| 5:P:633:LEU:HD21    | 5:P:647:LEU:CD1     | 2.10                     | 0.81              |
| 7:Q:221:TRP:CZ3     | 7:Q:222:PHE:HE2     | 1.97                     | 0.81              |
| 5:P8:506:ASN:ND2    | 7:Q8:153:GLU:OE1    | 2.13                     | 0.81              |
| 5:P16:42:SER:HA     | 6:O16:287:GLU:OE2   | 1.79                     | 0.81              |
| 10:C16:417:LEU:HB3  | 10:C16:472:ASN:ND2  | 1.94                     | 0.81              |
| 10:C16:586:PRO:HD2  | 10:C16:650:ARG:HH12 | 1.41                     | 0.81              |
| 11:A24:696:ILE:CD1  | 11:A24:728:ILE:HD12 | 2.09                     | 0.81              |
| 10:C24:390:HIS:NE2  | 10:C24:449:GLU:OE2  | 2.12                     | 0.81              |
| 10:C24:572:ILE:CD1  | 10:C24:606:MET:HE1  | 2.08                     | 0.81              |
| 10:C24:1560:GLN:OE1 | 10:C24:1601:TYR:CD1 | 2.34                     | 0.81              |
| 14:W:351:CYS:SG     | 14:W:447:MET:HE1    | 2.20                     | 0.81              |
| 10:C:1290:HIS:CD2   | 10:C:1334:MET:HE2   | 2.14                     | 0.81              |
| 10:C8:556:VAL:CG1   | 10:C8:565:ARG:HH22  | 1.90                     | 0.81              |
| 11:A32:54:ASN:HB3   | 11:A32:59:GLN:HE22  | 1.45                     | 0.81              |
| 22:I16:290:ASP:OD1  | 22:I16:293:LYS:HE3  | 1.80                     | 0.81              |
| 10:C32:110:ARG:HH11 | 10:C32:118:LEU:HD11 | 1.00                     | 0.81              |
| 10:C32:1560:GLN:OE1 | 10:C32:1601:TYR:CD1 | 2.34                     | 0.81              |
| 1:R:1132:TYR:CE1    | 1:R:1214:ILE:CD1    | 2.63                     | 0.81              |
| 1:R:1324:ASP:N      | 10:C:1154:TRP:HB2   | 1.95                     | 0.81              |
| 1:R:1424:LYS:HZ3    | 6:O:105:ASN:ND2     | 1.74                     | 0.81              |
| 2:M:225:ASP:HB3     | 2:M:606:GLN:HE21    | 1.45                     | 0.81              |
| 2:M8:593:HIS:CD2    | 3:N8:224:LEU:HD22   | 2.15                     | 0.81              |
| 4:T16:674:GLN:OE1   | 5:P16:695:GLN:CD    | 2.23                     | 0.81              |
| 5:P:251:LYS:HZ1     | 14:W:765:LYS:HZ3    | 0.84                     | 0.81              |
| 5:P:322:CYS:HB2     | 13:V:767:GLU:CD     | 2.05                     | 0.81              |
| 5:P:401:ARG:CD      | 5:P:414:VAL:CG2     | 2.33                     | 0.81              |
| 5:P16:187:TRP:CH2   | 5:P16:191:ARG:HD3   | 2.16                     | 0.81              |
| 6:O16:119:ARG:NH2   | 6:O16:182:GLU:CG    | 2.40                     | 0.81              |
| 7:Q16:149:VAL:HG23  | 7:Q16:187:TRP:CZ2   | 2.14                     | 0.81              |
| 8:L:621:SER:HB3     | 8:L:657:TYR:CE1     | 2.15                     | 0.81              |
| 9:K:1053:MET:O      | 9:K:1054:THR:C      | 2.12                     | 0.81              |
| 10:C16:843:MET:HE3  | 10:C16:911:ILE:HG12 | 1.60                     | 0.81              |
| 12:A:707:LEU:CD2    | 12:A:767:ARG:NH2    | 2.43                     | 0.81              |
| 19:4:183:ARG:NH2    | 19:4:242:VAL:O      | 2.13                     | 0.81              |
| 21:H:247:GLU:OE2    | 22:I:181:LEU:HD23   | 1.80                     | 0.81              |
| 22:I:199:PHE:CG     | 23:J32:620:MET:SD   | 2.73                     | 0.81              |
| 22:I8:199:PHE:CG    | 23:J8:620:MET:SD    | 2.73                     | 0.81              |
| 22:I16:199:PHE:CG   | 23:J16:620:MET:SD   | 2.73                     | 0.81              |
| 24:D8:857:THR:CG2   | 24:D8:885:TYR:HH    | 1.89                     | 0.81              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 24:D40:839:GLU:CB   | 24:D40:971:HIS:NE2   | 2.40                     | 0.81              |
| 24:D40:854:GLU:OE1  | 24:D40:927:GLN:CD    | 2.23                     | 0.81              |
| 1:R8:1381:GLU:O     | 1:R8:1382:LYS:CG     | 2.27                     | 0.81              |
| 2:M16:552:PHE:HZ    | 2:M16:559:PHE:HE2    | 1.28                     | 0.81              |
| 2:M16:627:TYR:HE1   | 3:N16:162:THR:HG21   | 1.46                     | 0.81              |
| 5:P8:47:ASN:OD1     | 5:P8:471:SER:OG      | 1.99                     | 0.81              |
| 5:P16:604:TYR:CE2   | 5:P16:629:ARG:NH2    | 2.48                     | 0.81              |
| 7:Q16:297:VAL:HG12  | 7:Q16:301:ARG:HB2    | 1.58                     | 0.81              |
| 9:K:853:ALA:CB      | 9:K:856:ILE:HD12     | 2.10                     | 0.81              |
| 9:K8:1085:TYR:CZ    | 9:K8:1093:SER:CB     | 2.64                     | 0.81              |
| 10:C16:837:ARG:CZ   | 10:C16:890:ASP:HB3   | 2.11                     | 0.81              |
| 10:C24:1430:ARG:HG3 | 10:C24:1482:MET:HE2  | 1.60                     | 0.81              |
| 10:C:847:ARG:NE     | 10:C:903:ASN:OD1     | 2.12                     | 0.81              |
| 10:C8:65:PRO:HG2    | 10:C8:96:ARG:HH22    | 1.42                     | 0.81              |
| 11:A16:90:PHE:CE1   | 18:B:1788:ILE:HG22   | 2.13                     | 0.81              |
| 11:A16:440:LEU:HB3  | 11:A16:443:LEU:HD12  | 1.57                     | 0.81              |
| 11:A32:703:ALA:CB   | 24:D32:1398:ARG:HH11 | 1.94                     | 0.81              |
| 18:B8:268:GLN:NE2   | 18:B8:323:GLU:HB3    | 1.96                     | 0.81              |
| 20:E:52:VAL:HG11    | 20:E:121:VAL:HG21    | 1.62                     | 0.81              |
| 24:D:1385:MET:SD    | 24:D:1464:PHE:CZ     | 2.73                     | 0.81              |
| 24:D24:857:THR:CB   | 24:D24:885:TYR:OH    | 2.25                     | 0.81              |
| 1:R:1424:LYS:HZ1    | 6:O:134:ARG:NH2      | 1.79                     | 0.81              |
| 2:M:625:HIS:HA      | 3:N:165:GLY:CA       | 2.10                     | 0.81              |
| 2:M8:820:LEU:HD13   | 2:M8:820:LEU:C       | 2.06                     | 0.81              |
| 1:R16:1125:ARG:NH2  | 2:M16:834:ASP:OD2    | 2.13                     | 0.81              |
| 5:P8:42:SER:HA      | 6:O8:287:GLU:OE2     | 1.79                     | 0.81              |
| 5:P8:614:VAL:CB     | 5:P8:629:ARG:NH1     | 2.25                     | 0.81              |
| 5:P16:645:LEU:HD21  | 5:P16:697:VAL:HG22   | 1.62                     | 0.81              |
| 9:K:847:LEU:HD21    | 9:K:910:SER:CB       | 2.09                     | 0.81              |
| 10:C16:75:GLN:HE21  | 10:C16:112:PRO:HG3   | 1.46                     | 0.81              |
| 10:C16:578:LEU:HB3  | 10:C16:584:ILE:HD13  | 1.62                     | 0.81              |
| 10:C16:663:ILE:HG22 | 10:C16:667:ILE:HD12  | 1.62                     | 0.81              |
| 13:V:818:THR:HG23   | 13:V:824:TRP:NE1     | 1.94                     | 0.81              |
| 14:W:781:LEU:CD2    | 15:J:695:ILE:HG21    | 2.11                     | 0.81              |
| 10:C:643:LEU:HD21   | 10:C:675:ASP:CG      | 2.03                     | 0.81              |
| 10:C:837:ARG:CZ     | 10:C:890:ASP:HB3     | 2.11                     | 0.81              |
| 18:B:671:MET:CE     | 18:B:736:ALA:HB2     | 2.09                     | 0.81              |
| 18:B8:618:VAL:HG12  | 18:B8:621:VAL:HG23   | 1.60                     | 0.81              |
| 19:4:189:LEU:CD1    | 19:4:203:LEU:CD2     | 2.50                     | 0.81              |
| 23:J24:686:MET:HE1  | 23:J24:694:ARG:HH21  | 1.43                     | 0.81              |
| 24:D8:1452:LYS:HZ1  | 24:D16:971:HIS:CE1   | 1.98                     | 0.81              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A48:440:LEU:CB   | 12:A48:443:LEU:HD11 | 2.07                     | 0.81              |
| 1:R:1059:ILE:CG2    | 24:D:1448:TYR:OH    | 2.28                     | 0.81              |
| 1:R8:982:GLU:OE1    | 24:D40:1436:ARG:NE  | 2.12                     | 0.81              |
| 1:R8:1165:MET:CE    | 1:R8:1220:GLN:HG2   | 2.10                     | 0.81              |
| 1:R16:1165:MET:CE   | 1:R16:1220:GLN:HG2  | 2.10                     | 0.81              |
| 5:P:633:LEU:CD2     | 5:P:639:THR:HG21    | 2.11                     | 0.81              |
| 5:P16:47:ASN:OD1    | 5:P16:471:SER:OG    | 1.99                     | 0.81              |
| 7:Q16:98:MET:HE2    | 7:Q16:110:VAL:CG1   | 2.10                     | 0.81              |
| 8:L16:853:MET:O     | 8:L16:1026:ARG:NH1  | 2.13                     | 0.81              |
| 10:C16:65:PRO:HG2   | 10:C16:96:ARG:HH22  | 1.42                     | 0.81              |
| 11:A40:798:PHE:HE1  | 11:A40:847:ARG:CZ   | 1.90                     | 0.81              |
| 13:V:758:CYS:O      | 13:V:762:LEU:HD12   | 1.80                     | 0.81              |
| 10:C:75:GLN:HE21    | 10:C:112:PRO:HG3    | 1.46                     | 0.81              |
| 10:C8:453:LEU:HD22  | 10:C8:459:LEU:HD22  | 1.60                     | 0.81              |
| 10:C8:837:ARG:CZ    | 10:C8:890:ASP:HB3   | 2.11                     | 0.81              |
| 11:A32:270:VAL:HG12 | 11:A32:274:MET:HB3  | 1.63                     | 0.81              |
| 18:B:1618:HIS:HE1   | 18:B:1622:ILE:HD11  | 1.39                     | 0.81              |
| 19:48:313:LEU:HD21  | 19:48:322:LEU:HD13  | 1.63                     | 0.81              |
| 24:D32:642:VAL:HG22 | 24:D40:631:ARG:NE   | 1.94                     | 0.81              |
| 1:R8:768:LEU:HD12   | 24:D40:1364:PRO:HD2 | 1.60                     | 0.81              |
| 1:R8:1442:THR:HG21  | 3:N8:13:ILE:HD12    | 1.63                     | 0.81              |
| 1:R16:1139:ARG:HG3  | 1:R16:1157:ARG:NH1  | 1.96                     | 0.81              |
| 1:R16:1223:PHE:CG   | 5:P16:676:GLN:NE2   | 2.48                     | 0.81              |
| 4:T16:671:ILE:CD1   | 5:P16:699:SER:N     | 2.43                     | 0.81              |
| 8:L16:1068:PHE:O    | 8:L16:1068:PHE:HD1  | 1.63                     | 0.81              |
| 10:C16:1560:GLN:OE1 | 10:C16:1601:TYR:CD1 | 2.34                     | 0.81              |
| 11:A24:798:PHE:HE1  | 11:A24:847:ARG:CZ   | 1.90                     | 0.81              |
| 10:C24:452:LEU:HD13 | 10:C24:452:LEU:C    | 2.04                     | 0.81              |
| 14:W:711:ARG:HB2    | 10:C8:1609:ASP:OD2  | 1.80                     | 0.81              |
| 10:C8:453:LEU:CD1   | 10:C8:486:LEU:HD21  | 2.11                     | 0.81              |
| 10:C8:653:TYR:OH    | 10:C8:679:ARG:HB3   | 1.78                     | 0.81              |
| 10:C8:653:TYR:CE1   | 10:C8:679:ARG:HD3   | 2.15                     | 0.81              |
| 18:B:1161:LEU:HD21  | 18:B:1403:ILE:HD12  | 1.63                     | 0.81              |
| 19:4:250:ILE:CD1    | 20:E:165:ARG:NH2    | 2.43                     | 0.81              |
| 10:C32:1271:PHE:HZ  | 10:C32:1284:ASP:CG  | 1.75                     | 0.81              |
| 10:C32:1790:GLN:O   | 10:C32:1794:THR:OG1 | 1.98                     | 0.81              |
| 1:R:1124:TRP:CZ2    | 4:T:669:PRO:CG      | 2.61                     | 0.81              |
| 1:R:1425:PRO:HA     | 6:O:165:LYS:CE      | 2.10                     | 0.81              |
| 5:P8:175:MET:SD     | 5:P8:433:LEU:HD22   | 2.21                     | 0.81              |
| 5:P8:510:ILE:CD1    | 7:Q8:183:ARG:HH12   | 1.93                     | 0.81              |
| 5:P8:611:LEU:C      | 5:P8:629:ARG:NH2    | 2.36                     | 0.81              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:P16:510:ILE:CD1   | 7:Q16:183:ARG:HH12  | 1.93                     | 0.81              |
| 9:K:792:LEU:HD12    | 9:K:864:ILE:CG1     | 2.11                     | 0.81              |
| 9:K8:1048:GLN:OE1   | 9:K8:1128:ARG:CG    | 2.29                     | 0.81              |
| 10:C16:758:GLN:NE2  | 10:C16:819:GLN:HG2  | 1.96                     | 0.81              |
| 10:C24:75:GLN:HE21  | 10:C24:112:PRO:HG3  | 1.46                     | 0.81              |
| 10:C24:110:ARG:HH11 | 10:C24:118:LEU:HD11 | 1.00                     | 0.81              |
| 10:C24:586:PRO:HD2  | 10:C24:650:ARG:HH12 | 1.41                     | 0.81              |
| 10:C24:670:GLU:O    | 10:C24:671:LYS:N    | 2.14                     | 0.81              |
| 10:C24:1708:ARG:NH2 | 21:H24:275:LYS:CD   | 2.43                     | 0.81              |
| 11:A40:707:LEU:CD2  | 11:A40:767:ARG:NH2  | 2.43                     | 0.81              |
| 12:A:440:LEU:CB     | 12:A:443:LEU:HD11   | 2.07                     | 0.81              |
| 10:C:670:GLU:O      | 10:C:671:LYS:N      | 2.14                     | 0.81              |
| 10:C8:1619:PRO:C    | 10:C8:1621:LYS:H    | 1.89                     | 0.81              |
| 18:B:86:LYS:HE2     | 18:B:123:LEU:CD1    | 2.10                     | 0.81              |
| 18:B8:1161:LEU:HD21 | 18:B8:1403:ILE:HD12 | 1.63                     | 0.81              |
| 19:48:189:LEU:HD22  | 19:48:203:LEU:HD23  | 1.63                     | 0.81              |
| 24:D40:839:GLU:OE2  | 24:D40:971:HIS:HB3  | 1.78                     | 0.81              |
| 7:Q16:187:TRP:HH2   | 7:Q16:207:GLN:HE22  | 1.29                     | 0.81              |
| 8:L:1077:LEU:HD13   | 9:K:1086:VAL:CG1    | 2.10                     | 0.81              |
| 10:C24:249:THR:C    | 10:C24:251:GLY:N    | 2.37                     | 0.81              |
| 10:C24:663:ILE:HG22 | 10:C24:667:ILE:HD12 | 1.62                     | 0.81              |
| 10:C24:1271:PHE:HZ  | 10:C24:1284:ASP:CG  | 1.75                     | 0.81              |
| 12:A:270:VAL:HG12   | 12:A:274:MET:HB3    | 1.63                     | 0.81              |
| 10:C:407:LYS:HZ2    | 10:C:465:PHE:HE2    | 1.28                     | 0.81              |
| 10:C:1560:GLN:OE1   | 10:C:1601:TYR:CD1   | 2.34                     | 0.81              |
| 20:E8:432:ILE:HD13  | 24:D40:72:GLU:HG3   | 1.23                     | 0.81              |
| 24:D24:857:THR:CG2  | 24:D24:889:LEU:HD13 | 2.11                     | 0.81              |
| 10:C32:65:PRO:HG2   | 10:C32:96:ARG:HH22  | 1.42                     | 0.81              |
| 10:C32:758:GLN:NE2  | 10:C32:819:GLN:HG2  | 1.96                     | 0.81              |
| 12:A48:273:ARG:HE   | 12:A48:479:LEU:HD23 | 1.42                     | 0.81              |
| 2:M:672:TYR:HB2     | 2:M:680:LYS:HD3     | 1.61                     | 0.81              |
| 1:R16:1124:TRP:CZ3  | 1:R16:1170:LEU:O    | 2.34                     | 0.81              |
| 2:M16:820:LEU:HD13  | 2:M16:820:LEU:C     | 2.06                     | 0.81              |
| 7:Q:98:MET:HE2      | 7:Q:110:VAL:CG1     | 2.10                     | 0.81              |
| 8:L16:177:ARG:CG    | 12:A48:744:GLU:CD   | 2.46                     | 0.81              |
| 9:K8:1180:TRP:CG    | 9:K8:1261:MET:HE2   | 2.16                     | 0.81              |
| 10:C16:390:HIS:CD2  | 10:C16:452:LEU:CG   | 2.57                     | 0.81              |
| 10:C16:390:HIS:CE1  | 10:C16:449:GLU:CB   | 2.50                     | 0.81              |
| 10:C16:670:GLU:O    | 10:C16:671:LYS:N    | 2.14                     | 0.81              |
| 10:C16:1547:LYS:NZ  | 24:D8:1405:GLY:H    | 1.79                     | 0.81              |
| 10:C16:1688:ARG:HG3 | 23:J32:735:LYS:HE2  | 1.63                     | 0.81              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:758:GLN:NE2  | 10:C24:819:GLN:HG2   | 1.96                     | 0.81              |
| 10:C24:843:MET:HE3  | 10:C24:911:ILE:HG12  | 1.61                     | 0.81              |
| 10:C24:1010:ALA:CA  | 10:C24:1192:ARG:HH21 | 1.92                     | 0.81              |
| 14:W:638:VAL:CG1    | 15:J:561:PHE:HZ      | 1.93                     | 0.81              |
| 10:C:578:LEU:HB3    | 10:C:584:ILE:HD13    | 1.62                     | 0.81              |
| 10:C:663:ILE:HG22   | 10:C:667:ILE:HD12    | 1.62                     | 0.81              |
| 11:A32:698:LYS:HD3  | 11:A32:804:TYR:HE1   | 1.46                     | 0.81              |
| 18:B:13:TRP:O       | 18:B:107:ARG:NH2     | 2.12                     | 0.81              |
| 18:B8:1279:THR:OG1  | 18:B8:1289:ASP:OD1   | 1.99                     | 0.81              |
| 22:I:146:SER:OG     | 23:J32:574:ARG:NH1   | 2.13                     | 0.81              |
| 10:C32:837:ARG:CZ   | 10:C32:890:ASP:HB3   | 2.11                     | 0.81              |
| 12:A48:270:VAL:HG12 | 12:A48:274:MET:HB3   | 1.62                     | 0.81              |
| 1:R:1425:PRO:HA     | 6:O:165:LYS:HZ1      | 1.00                     | 0.80              |
| 2:M8:833:GLU:OE1    | 4:T8:667:ILE:CA      | 2.27                     | 0.80              |
| 2:M16:627:TYR:CE1   | 3:N16:162:THR:HG21   | 2.16                     | 0.80              |
| 5:P:506:ASN:ND2     | 7:Q:153:GLU:OE1      | 2.13                     | 0.80              |
| 5:P16:105:ARG:CZ    | 5:P16:133:TYR:CD1    | 2.63                     | 0.80              |
| 8:L8:1074:ARG:CD    | 9:K8:1089:LYS:HG2    | 2.09                     | 0.80              |
| 8:L8:1074:ARG:HB3   | 9:K8:1089:LYS:HE2    | 1.61                     | 0.80              |
| 10:C16:1790:GLN:O   | 10:C16:1794:THR:OG1  | 1.98                     | 0.80              |
| 10:C24:837:ARG:CZ   | 10:C24:890:ASP:HB3   | 2.11                     | 0.80              |
| 11:A16:706:SER:HB3  | 24:D16:1398:ARG:HG2  | 1.62                     | 0.80              |
| 18:B:856:LEU:HD23   | 18:B:860:HIS:CB      | 2.10                     | 0.80              |
| 18:B:1152:ASP:OD2   | 18:B:1378:LYS:NZ     | 2.15                     | 0.80              |
| 18:B8:1152:ASP:OD2  | 18:B8:1378:LYS:NZ    | 2.15                     | 0.80              |
| 19:4:189:LEU:HD22   | 19:4:203:LEU:HD23    | 1.63                     | 0.80              |
| 20:E8:352:PHE:HE1   | 20:E8:451:ILE:HD13   | 1.03                     | 0.80              |
| 24:D:1435:ARG:NH1   | 24:D:1448:TYR:CE2    | 2.21                     | 0.80              |
| 10:C32:64:LEU:HD12  | 10:C32:70:ILE:HD12   | 1.63                     | 0.80              |
| 10:C32:453:LEU:CD1  | 10:C32:486:LEU:HD21  | 2.11                     | 0.80              |
| 1:R:1266:THR:HA     | 5:P:684:ARG:HH21     | 1.45                     | 0.80              |
| 2:M:762:LEU:CB      | 2:M:813:ASN:HD22     | 1.83                     | 0.80              |
| 2:M:833:GLU:OE1     | 4:T:667:ILE:CA       | 2.27                     | 0.80              |
| 1:R8:1124:TRP:CZ3   | 1:R8:1170:LEU:O      | 2.35                     | 0.80              |
| 2:M8:816:ARG:HH12   | 2:M8:849:LEU:C       | 1.88                     | 0.80              |
| 2:M8:816:ARG:NH1    | 2:M8:850:TYR:N       | 2.30                     | 0.80              |
| 2:M16:202:LYS:HZ2   | 2:M16:208:SER:C      | 1.87                     | 0.80              |
| 2:M16:816:ARG:NH1   | 2:M16:850:TYR:N      | 2.30                     | 0.80              |
| 5:P:47:ASN:OD1      | 5:P:471:SER:OG       | 1.99                     | 0.80              |
| 10:C16:390:HIS:CD2  | 10:C16:452:LEU:CD1   | 2.64                     | 0.80              |
| 10:C24:1699:LYS:CE  | 23:J24:722:LEU:HD22  | 2.11                     | 0.80              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 14:W:638:VAL:HG11    | 15:J:561:PHE:HZ     | 1.39                     | 0.80              |
| 10:C:1163:LEU:CD2    | 10:C:1166:SER:OG    | 2.30                     | 0.80              |
| 18:B:618:VAL:HG12    | 18:B:621:VAL:HG23   | 1.60                     | 0.80              |
| 18:B:1264:GLN:NE2    | 18:B:1394:TRP:CZ3   | 2.49                     | 0.80              |
| 19:4:97:LEU:HD21     | 19:4:232:TYR:CG     | 2.15                     | 0.80              |
| 19:48:97:LEU:HD21    | 19:48:232:TYR:CG    | 2.15                     | 0.80              |
| 10:C32:249:THR:C     | 10:C32:251:GLY:N    | 2.37                     | 0.80              |
| 1:R:1442:THR:HG21    | 3:N:13:ILE:HD12     | 1.63                     | 0.80              |
| 3:N16:19:MET:CE      | 3:N16:23:GLY:C      | 2.51                     | 0.80              |
| 8:L:1089:MET:HE1     | 9:K:1004:ARG:HE     | 1.46                     | 0.80              |
| 9:K8:792:LEU:HG      | 9:K8:864:ILE:HD11   | 1.62                     | 0.80              |
| 10:C16:407:LYS:HZ2   | 10:C16:465:PHE:HE2  | 1.28                     | 0.80              |
| 10:C16:1661:LEU:HD23 | 10:C24:1565:GLN:HG3 | 1.64                     | 0.80              |
| 13:V:815:TYR:OH      | 15:J:627:ILE:HD12   | 1.80                     | 0.80              |
| 11:A16:112:ALA:CB    | 18:B:1416:LYS:HZ1   | 1.94                     | 0.80              |
| 11:A32:703:ALA:O     | 24:D32:1398:ARG:CZ  | 2.29                     | 0.80              |
| 18:B:1669:PRO:HG3    | 18:B:1748:HIS:CD2   | 2.16                     | 0.80              |
| 18:B8:493:VAL:HG11   | 18:B8:520:ILE:HD13  | 1.61                     | 0.80              |
| 18:B8:729:LEU:CD1    | 18:B8:1196:MET:HE1  | 2.11                     | 0.80              |
| 18:B8:856:LEU:HD23   | 18:B8:860:HIS:CB    | 2.10                     | 0.80              |
| 21:H:366:MET:HE1     | 22:I:332:MET:HE3    | 1.62                     | 0.80              |
| 22:I8:290:ASP:OD1    | 22:I8:293:LYS:HE3   | 1.80                     | 0.80              |
| 22:I24:131:ARG:CD    | 23:J24:557:ARG:NH2  | 2.44                     | 0.80              |
| 22:I24:146:SER:OG    | 23:J24:574:ARG:NH1  | 2.13                     | 0.80              |
| 24:D24:342:LEU:HD11  | 24:D24:348:MET:HE3  | 1.63                     | 0.80              |
| 2:M16:833:GLU:OE1    | 4:T16:667:ILE:CA    | 2.27                     | 0.80              |
| 5:P8:645:LEU:HD21    | 5:P8:697:VAL:HG22   | 1.63                     | 0.80              |
| 9:K:1248:LEU:CD1     | 9:K:1265:ILE:HD12   | 2.11                     | 0.80              |
| 9:K8:955:TYR:CE1     | 9:K8:985:PHE:CB     | 2.63                     | 0.80              |
| 10:C16:1430:ARG:HG3  | 10:C16:1482:MET:HE2 | 1.60                     | 0.80              |
| 11:A24:737:GLU:CD    | 24:D16:871:ARG:HE   | 1.88                     | 0.80              |
| 10:C24:386:ASN:O     | 10:C24:390:HIS:CD2  | 2.35                     | 0.80              |
| 11:A40:270:VAL:HG12  | 11:A40:274:MET:HB3  | 1.62                     | 0.80              |
| 10:C:758:GLN:NE2     | 10:C:819:GLN:HG2    | 1.96                     | 0.80              |
| 10:C8:556:VAL:HG12   | 10:C8:565:ARG:NH2   | 1.96                     | 0.80              |
| 10:C8:1560:GLN:OE1   | 10:C8:1601:TYR:CD1  | 2.34                     | 0.80              |
| 11:A32:703:ALA:HB1   | 24:D32:1398:ARG:NH1 | 1.95                     | 0.80              |
| 18:B:65:LEU:HD23     | 18:B:79:ILE:HD12    | 1.62                     | 0.80              |
| 18:B:1101:TYR:CE1    | 18:B:1105:LEU:HD11  | 2.17                     | 0.80              |
| 18:B8:1669:PRO:HG3   | 18:B8:1748:HIS:CD2  | 2.16                     | 0.80              |
| 20:E8:52:VAL:HG11    | 20:E8:121:VAL:HG21  | 1.62                     | 0.80              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 24:D24:853:MET:HB3   | 24:D24:885:TYR:CE2  | 2.16                     | 0.80              |
| 1:R:1124:TRP:CZ3     | 1:R:1170:LEU:O      | 2.35                     | 0.80              |
| 1:R:1424:LYS:HZ1     | 6:O:105:ASN:ND2     | 1.78                     | 0.80              |
| 2:M:820:LEU:HD13     | 2:M:820:LEU:C       | 2.05                     | 0.80              |
| 2:M8:627:TYR:HD2     | 3:N8:167:LEU:HA     | 1.44                     | 0.80              |
| 2:M16:202:LYS:HE3    | 2:M16:206:SER:OG    | 1.81                     | 0.80              |
| 6:O16:82:LEU:CD2     | 6:O16:103:MET:CE    | 2.59                     | 0.80              |
| 9:K:919:MET:SD       | 9:K:938:PHE:CD2     | 2.75                     | 0.80              |
| 9:K:1085:TYR:CZ      | 9:K:1093:SER:CB     | 2.64                     | 0.80              |
| 9:K8:1248:LEU:CD1    | 9:K8:1265:ILE:HD12  | 2.10                     | 0.80              |
| 11:A24:212:LYS:HE2   | 11:A24:585:MET:HE1  | 0.80                     | 0.80              |
| 11:A24:390:ALA:HB2   | 24:D16:1099:ARG:HB2 | 1.63                     | 0.80              |
| 10:C24:565:ARG:CD    | 10:C24:568:TRP:HE3  | 1.91                     | 0.80              |
| 14:W:715:ASP:HA      | 10:C8:1568:ARG:HH11 | 1.00                     | 0.80              |
| 10:C:453:LEU:CD1     | 10:C:486:LEU:HD21   | 2.11                     | 0.80              |
| 18:B:583:ARG:NH1     | 18:B:711:CYS:CB     | 2.43                     | 0.80              |
| 19:48:250:ILE:CB     | 20:E8:165:ARG:HH22  | 1.95                     | 0.80              |
| 22:I:131:ARG:CD      | 23:J32:557:ARG:NH2  | 2.44                     | 0.80              |
| 22:I8:146:SER:OG     | 23:J8:574:ARG:NH1   | 2.13                     | 0.80              |
| 21:H16:247:GLU:OE2   | 22:I16:181:LEU:CD2  | 2.30                     | 0.80              |
| 10:C32:578:LEU:HB3   | 10:C32:584:ILE:HD13 | 1.62                     | 0.80              |
| 2:M16:377:ARG:CZ     | 2:M16:477:ASP:HB3   | 2.12                     | 0.80              |
| 5:P:401:ARG:HD3      | 5:P:414:VAL:HG21    | 1.63                     | 0.80              |
| 5:P:645:LEU:HD21     | 5:P:697:VAL:HG22    | 1.62                     | 0.80              |
| 7:Q8:187:TRP:HH2     | 7:Q8:207:GLN:HE22   | 1.29                     | 0.80              |
| 9:K:1180:TRP:CG      | 9:K:1261:MET:HE2    | 2.17                     | 0.80              |
| 10:C16:1619:PRO:C    | 10:C16:1621:LYS:H   | 1.89                     | 0.80              |
| 11:A24:607:ARG:HH22  | 24:D16:914:PHE:HD1  | 1.29                     | 0.80              |
| 10:C24:389:LEU:CD2   | 10:C24:447:PHE:CE1  | 2.60                     | 0.80              |
| 10:C24:453:LEU:CD1   | 10:C24:486:LEU:HD21 | 2.11                     | 0.80              |
| 10:C24:1708:ARG:HH21 | 21:H24:275:LYS:CE   | 1.94                     | 0.80              |
| 13:V:790:GLN:CD      | 14:W:674:GLN:HE22   | 1.90                     | 0.80              |
| 10:C8:670:GLU:O      | 10:C8:671:LYS:N     | 2.14                     | 0.80              |
| 11:A16:11:THR:HG21   | 22:I:162:GLN:HE21   | 1.47                     | 0.80              |
| 19:48:250:ILE:CD1    | 20:E8:165:ARG:NH2   | 2.43                     | 0.80              |
| 21:H8:247:GLU:OE2    | 22:I8:181:LEU:CD2   | 2.30                     | 0.80              |
| 21:H16:244:ARG:HH21  | 22:I16:177:VAL:HG13 | 1.47                     | 0.80              |
| 1:R16:1381:GLU:O     | 1:R16:1382:LYS:CG   | 2.28                     | 0.80              |
| 2:M16:627:TYR:HE1    | 3:N16:162:THR:CG2   | 1.95                     | 0.80              |
| 5:P:175:MET:HE1      | 5:P:436:ALA:HB2     | 1.64                     | 0.80              |
| 5:P8:187:TRP:CH2     | 5:P8:191:ARG:HD3    | 2.16                     | 0.80              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:O8:82:LEU:CD2     | 6:O8:103:MET:CE     | 2.59                     | 0.80              |
| 6:O8:164:GLY:O      | 6:O8:166:PRO:HD3    | 1.81                     | 0.80              |
| 9:K:959:TRP:CE2     | 9:K:992:GLN:HB3     | 2.16                     | 0.80              |
| 10:C24:1691:GLU:OE2 | 23:J24:735:LYS:HA   | 1.82                     | 0.80              |
| 11:A40:212:LYS:HE2  | 11:A40:585:MET:HE1  | 0.80                     | 0.80              |
| 13:V:861:PHE:HZ     | 14:W:742:VAL:HG22   | 1.47                     | 0.80              |
| 10:C:64:LEU:HD12    | 10:C:70:ILE:HD12    | 1.63                     | 0.80              |
| 10:C8:1790:GLN:O    | 10:C8:1794:THR:OG1  | 1.98                     | 0.80              |
| 11:A16:707:LEU:CD2  | 11:A16:767:ARG:NH2  | 2.43                     | 0.80              |
| 18:B:268:GLN:NE2    | 18:B:323:GLU:HB3    | 1.96                     | 0.80              |
| 21:H24:247:GLU:OE2  | 22:I24:181:LEU:CD2  | 2.30                     | 0.80              |
| 12:A48:707:LEU:CD2  | 12:A48:767:ARG:NH2  | 2.43                     | 0.80              |
| 1:R:1460:MET:HE3    | 1:R:1463:GLN:OE1    | 1.81                     | 0.80              |
| 5:P8:101:LEU:CD2    | 5:P8:133:TYR:CD2    | 2.65                     | 0.80              |
| 9:K:1048:GLN:HG3    | 9:K:1074:ARG:HH22   | 1.47                     | 0.80              |
| 10:C16:345:MET:HE3  | 10:C16:401:ILE:HD11 | 1.46                     | 0.80              |
| 10:C16:452:LEU:HD23 | 10:C16:452:LEU:H    | 1.44                     | 0.80              |
| 10:C24:1619:PRO:C   | 10:C24:1621:LYS:H   | 1.89                     | 0.80              |
| 13:V:825:GLN:HA     | 14:W:707:LYS:HZ2    | 1.46                     | 0.80              |
| 15:J:623:GLU:OE2    | 15:J:626:ARG:CZ     | 2.30                     | 0.80              |
| 10:C:18:THR:HG23    | 10:C:883:GLU:CG     | 2.12                     | 0.80              |
| 11:A16:557:LEU:CD2  | 11:A16:561:ASP:HB3  | 2.12                     | 0.80              |
| 18:B:493:VAL:HG11   | 18:B:520:ILE:HD13   | 1.61                     | 0.80              |
| 18:B:789:LEU:HD23   | 18:B:793:LEU:CD1    | 2.12                     | 0.80              |
| 18:B8:1205:ILE:HD11 | 18:B8:1271:PHE:HD2  | 1.43                     | 0.80              |
| 18:B8:1264:GLN:NE2  | 18:B8:1394:TRP:CZ3  | 2.50                     | 0.80              |
| 20:E:49:THR:HG23    | 20:E:121:VAL:CG1    | 2.11                     | 0.80              |
| 22:I8:131:ARG:CD    | 23:J8:557:ARG:NH2   | 2.44                     | 0.80              |
| 10:C32:670:GLU:O    | 10:C32:671:LYS:N    | 2.14                     | 0.80              |
| 10:C32:1619:PRO:C   | 10:C32:1621:LYS:H   | 1.89                     | 0.80              |
| 12:A48:312:LEU:CD1  | 12:A48:364:ILE:HD11 | 2.12                     | 0.80              |
| 2:M:399:THR:HB      | 2:M:480:ARG:HH21    | 1.47                     | 0.80              |
| 6:O:180:GLY:C       | 6:O:182:GLU:H       | 1.90                     | 0.80              |
| 5:P8:394:ASN:C      | 5:P8:396:SER:H      | 1.90                     | 0.80              |
| 10:C16:453:LEU:CD1  | 10:C16:486:LEU:HD21 | 2.11                     | 0.80              |
| 11:A24:270:VAL:HG12 | 11:A24:274:MET:HB3  | 1.62                     | 0.80              |
| 10:C:643:LEU:HD11   | 10:C:679:ARG:HH12   | 1.41                     | 0.80              |
| 10:C:1790:GLN:O     | 10:C:1794:THR:OG1   | 1.98                     | 0.80              |
| 11:A32:90:PHE:CE1   | 18:B8:1788:ILE:HG22 | 2.15                     | 0.80              |
| 20:E:473:LEU:HD23   | 20:E:480:MET:SD     | 2.22                     | 0.80              |
| 10:C32:565:ARG:NH1  | 10:C32:602:VAL:HG13 | 1.97                     | 0.80              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 9:K:916:LYS:HG2      | 9:K:919:MET:HE1     | 1.55                     | 0.80              |
| 10:C16:1074:LEU:HD12 | 10:C16:1074:LEU:C   | 2.06                     | 0.80              |
| 10:C24:1790:GLN:O    | 10:C24:1794:THR:OG1 | 1.98                     | 0.80              |
| 11:A40:312:LEU:CD1   | 11:A40:364:ILE:HD11 | 2.12                     | 0.80              |
| 13:V:745:LEU:HD13    | 15:J:557:ARG:NH1    | 1.97                     | 0.80              |
| 10:C:453:LEU:CD2     | 10:C:459:LEU:HD11   | 2.08                     | 0.80              |
| 10:C:1560:GLN:OE1    | 10:C:1601:TYR:CE1   | 2.35                     | 0.80              |
| 10:C8:64:LEU:HD12    | 10:C8:70:ILE:HD12   | 1.63                     | 0.80              |
| 11:A32:212:LYS:HE2   | 11:A32:585:MET:HE1  | 0.80                     | 0.80              |
| 11:A32:706:SER:CB    | 24:D32:1398:ARG:HG2 | 2.12                     | 0.80              |
| 18:B:460:PRO:HB2     | 18:B:562:ARG:NH1    | 1.97                     | 0.80              |
| 19:4:313:LEU:HD21    | 19:4:322:LEU:HD13   | 1.63                     | 0.80              |
| 19:48:332:PRO:HD3    | 20:E8:294:VAL:HG13  | 1.61                     | 0.80              |
| 22:I16:155:PHE:CE1   | 22:I16:159:ARG:HD2  | 2.17                     | 0.80              |
| 10:C32:390:HIS:CE1   | 10:C32:452:LEU:HD22 | 2.16                     | 0.80              |
| 10:C32:1624:LEU:HD23 | 10:C32:1628:SER:HB2 | 1.64                     | 0.80              |
| 2:M:816:ARG:NH1      | 2:M:850:TYR:N       | 2.30                     | 0.79              |
| 1:R8:1466:LYS:CD     | 6:O8:160:LEU:CD2    | 2.60                     | 0.79              |
| 5:P8:611:LEU:CA      | 5:P8:629:ARG:NH2    | 2.46                     | 0.79              |
| 6:O8:28:SER:OG       | 6:O8:30:ASN:OD1     | 2.00                     | 0.79              |
| 5:P16:497:LEU:HA     | 6:O16:290:MET:HE1   | 1.63                     | 0.79              |
| 9:K:788:LEU:HD23     | 9:K:856:ILE:HD11    | 1.64                     | 0.79              |
| 11:A24:156:MET:HG2   | 11:A24:555:HIS:CE1  | 1.93                     | 0.79              |
| 11:A24:312:LEU:CD1   | 11:A24:364:ILE:HD11 | 2.12                     | 0.79              |
| 10:C24:1708:ARG:NH2  | 21:H24:275:LYS:HE2  | 1.96                     | 0.79              |
| 12:A:798:PHE:HE1     | 12:A:847:ARG:CZ     | 1.91                     | 0.79              |
| 11:A32:11:THR:HG21   | 22:I24:162:GLN:HE21 | 1.47                     | 0.79              |
| 11:A32:312:LEU:CD1   | 11:A32:364:ILE:HD11 | 2.12                     | 0.79              |
| 11:A32:707:LEU:CD2   | 11:A32:767:ARG:NH2  | 2.43                     | 0.79              |
| 18:B:729:LEU:CD1     | 18:B:1196:MET:HE1   | 2.11                     | 0.79              |
| 20:E8:473:LEU:HD23   | 20:E8:480:MET:SD    | 2.22                     | 0.79              |
| 21:H16:366:MET:HE1   | 22:I16:332:MET:HE3  | 1.62                     | 0.79              |
| 10:C32:1163:LEU:CD2  | 10:C32:1166:SER:OG  | 2.29                     | 0.79              |
| 3:N8:263:TRP:HE1     | 3:N8:279:GLY:HA2    | 1.47                     | 0.79              |
| 1:R16:1139:ARG:HB2   | 1:R16:1157:ARG:CZ   | 2.12                     | 0.79              |
| 1:R16:1212:SER:OG    | 1:R16:1218:LYS:NZ   | 2.15                     | 0.79              |
| 5:P:187:TRP:CH2      | 5:P:191:ARG:HD3     | 2.15                     | 0.79              |
| 7:Q8:295:SER:C       | 7:Q8:297:VAL:H      | 1.91                     | 0.79              |
| 10:C16:110:ARG:HH11  | 10:C16:118:LEU:HD11 | 1.00                     | 0.79              |
| 10:C16:565:ARG:HD2   | 10:C16:568:TRP:CD2  | 2.17                     | 0.79              |
| 10:C16:1163:LEU:CD2  | 10:C16:1166:SER:OG  | 2.29                     | 0.79              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1499:ASN:OD1  | 10:C24:1661:LEU:HB2  | 1.82                     | 0.79              |
| 10:C24:345:MET:HE3   | 10:C24:401:ILE:HD13  | 1.49                     | 0.79              |
| 11:A40:557:LEU:CD2   | 11:A40:561:ASP:HB3   | 2.12                     | 0.79              |
| 10:C:386:ASN:O       | 10:C:390:HIS:CD2     | 2.34                     | 0.79              |
| 10:C8:758:GLN:NE2    | 10:C8:819:GLN:HG2    | 1.96                     | 0.79              |
| 11:A32:698:LYS:CE    | 24:D32:1393:GLY:HA2  | 2.12                     | 0.79              |
| 18:B8:719:GLU:OE2    | 18:B8:766:LYS:NZ     | 2.15                     | 0.79              |
| 18:B8:856:LEU:HD11   | 18:B8:907:SER:HB2    | 1.64                     | 0.79              |
| 21:H:247:GLU:OE2     | 22:I:181:LEU:CD2     | 2.30                     | 0.79              |
| 22:I16:131:ARG:CD    | 23:J16:557:ARG:NH2   | 2.44                     | 0.79              |
| 24:D40:342:LEU:HD11  | 24:D40:348:MET:HE3   | 1.63                     | 0.79              |
| 10:C32:75:GLN:HE21   | 10:C32:112:PRO:HG3   | 1.46                     | 0.79              |
| 10:C32:1250:ALA:HB2  | 10:C32:1309:ARG:HH12 | 1.48                     | 0.79              |
| 1:R:1190:VAL:HG21    | 24:D:1457:SER:HA     | 1.65                     | 0.79              |
| 2:M:417:ARG:CA       | 8:L:346:TRP:HZ2      | 1.96                     | 0.79              |
| 1:R8:1101:ARG:HD2    | 24:D40:1459:LEU:O    | 1.81                     | 0.79              |
| 1:R8:1381:GLU:O      | 1:R8:1382:LYS:HG3    | 1.82                     | 0.79              |
| 2:M16:672:TYR:CB     | 2:M16:680:LYS:HD3    | 2.12                     | 0.79              |
| 3:N16:263:TRP:HE1    | 3:N16:279:GLY:HA2    | 1.47                     | 0.79              |
| 7:Q8:27:GLN:HE22     | 7:Q8:33:ARG:HG2      | 1.45                     | 0.79              |
| 6:O16:164:GLY:O      | 6:O16:166:PRO:HD3    | 1.82                     | 0.79              |
| 10:C16:1335:ILE:O    | 10:C16:1337:LEU:N    | 2.16                     | 0.79              |
| 11:A24:390:ALA:HB1   | 24:D16:1099:ARG:CD   | 2.11                     | 0.79              |
| 10:C24:1283:LEU:HD23 | 10:C24:1287:MET:HG3  | 1.64                     | 0.79              |
| 11:A40:156:MET:HA    | 11:A40:555:HIS:HD2   | 1.43                     | 0.79              |
| 11:A40:445:ASN:CG    | 17:F16:65:ARG:NH1    | 2.28                     | 0.79              |
| 13:V:909:ALA:HB3     | 14:W:787:MET:HE2     | 1.63                     | 0.79              |
| 10:C:407:LYS:CG      | 10:C:465:PHE:HZ      | 1.94                     | 0.79              |
| 10:C:565:ARG:CD      | 10:C:568:TRP:HE3     | 1.92                     | 0.79              |
| 18:B:1121:ALA:O      | 18:B:1123:ASN:N      | 2.15                     | 0.79              |
| 18:B:1130:LEU:CD2    | 18:B:1132:TRP:HE1    | 1.93                     | 0.79              |
| 19:48:189:LEU:CD2    | 19:48:203:LEU:HD23   | 2.13                     | 0.79              |
| 22:I8:155:PHE:CE1    | 22:I8:159:ARG:HD2    | 2.17                     | 0.79              |
| 2:M:210:GLN:CD       | 10:C:529:GLN:HE21    | 1.89                     | 0.79              |
| 2:M:377:ARG:CZ       | 2:M:477:ASP:HB3      | 2.12                     | 0.79              |
| 2:M16:399:THR:HB     | 2:M16:480:ARG:HH21   | 1.47                     | 0.79              |
| 9:K:695:GLU:OE1      | 9:K:820:TYR:OH       | 2.00                     | 0.79              |
| 9:K:1048:GLN:OE1     | 9:K:1128:ARG:CG      | 2.29                     | 0.79              |
| 9:K8:1049:ASP:O      | 9:K8:1050:GLU:C      | 2.13                     | 0.79              |
| 10:C24:278:ARG:NH1   | 10:C24:327:ILE:HG23  | 1.98                     | 0.79              |
| 10:C24:565:ARG:HD2   | 10:C24:568:TRP:CD2   | 2.17                     | 0.79              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C24:1163:LEU:CD2  | 10:C24:1166:SER:OG  | 2.30                     | 0.79              |
| 12:A:212:LYS:HE2     | 12:A:585:MET:HE1    | 0.80                     | 0.79              |
| 10:C:565:ARG:HD2     | 10:C:568:TRP:CD2    | 2.17                     | 0.79              |
| 10:C:1250:ALA:HB2    | 10:C:1309:ARG:HH12  | 1.47                     | 0.79              |
| 10:C8:249:THR:C      | 10:C8:251:GLY:N     | 2.36                     | 0.79              |
| 10:C8:1560:GLN:OE1   | 10:C8:1601:TYR:CE1  | 2.35                     | 0.79              |
| 10:C8:1624:LEU:HD23  | 10:C8:1628:SER:HB2  | 1.65                     | 0.79              |
| 17:F24:74:ILE:C      | 17:F24:76:ASP:N     | 2.38                     | 0.79              |
| 18:B:1130:LEU:CD2    | 18:B:1132:TRP:NE1   | 2.45                     | 0.79              |
| 18:B8:460:PRO:HB2    | 18:B8:562:ARG:NH1   | 1.97                     | 0.79              |
| 18:B8:1121:ALA:O     | 18:B8:1123:ASN:N    | 2.15                     | 0.79              |
| 18:B8:1161:LEU:CD2   | 18:B8:1164:GLU:OE2  | 2.31                     | 0.79              |
| 22:I:290:ASP:OD1     | 22:I:293:LYS:HE3    | 1.80                     | 0.79              |
| 21:H16:312:GLN:CG    | 21:H16:316:ILE:CD1  | 2.39                     | 0.79              |
| 10:C32:1283:LEU:HD23 | 10:C32:1287:MET:HG3 | 1.64                     | 0.79              |
| 10:C32:1285:VAL:HG21 | 10:C32:1738:MET:HE3 | 1.61                     | 0.79              |
| 10:C32:1466:ARG:NH1  | 12:A48:127:SER:OG   | 2.16                     | 0.79              |
| 1:R:1381:GLU:O       | 1:R:1382:LYS:HG3    | 1.82                     | 0.79              |
| 7:Q:187:TRP:HH2      | 7:Q:207:GLN:HE22    | 1.29                     | 0.79              |
| 8:L8:1064:ASP:OD2    | 9:K8:1101:GLU:OE1   | 1.99                     | 0.79              |
| 9:K8:1214:TYR:CB     | 9:K8:1269:CYS:SG    | 2.71                     | 0.79              |
| 10:C24:64:LEU:HD12   | 10:C24:70:ILE:HD12  | 1.63                     | 0.79              |
| 10:C24:1466:ARG:NH1  | 11:A40:127:SER:OG   | 2.16                     | 0.79              |
| 10:C:565:ARG:HH22    | 10:C:569:PHE:HD2    | 1.28                     | 0.79              |
| 10:C8:578:LEU:HB3    | 10:C8:584:ILE:HD13  | 1.63                     | 0.79              |
| 10:C8:639:MET:O      | 10:C8:643:LEU:HD13  | 1.82                     | 0.79              |
| 18:B:1045:LYS:HZ1    | 18:B:1100:LEU:CD2   | 1.95                     | 0.79              |
| 18:B:1161:LEU:CD2    | 18:B:1164:GLU:OE2   | 2.31                     | 0.79              |
| 20:E8:432:ILE:HB     | 24:D40:72:GLU:HG2   | 1.65                     | 0.79              |
| 22:I:131:ARG:NE      | 23:J32:557:ARG:NH2  | 2.31                     | 0.79              |
| 22:I:155:PHE:CE1     | 22:I:159:ARG:HD2    | 2.17                     | 0.79              |
| 24:D40:873:ARG:HH11  | 24:D40:884:ASP:HB3  | 0.99                     | 0.79              |
| 10:C32:1335:ILE:O    | 10:C32:1337:LEU:N   | 2.16                     | 0.79              |
| 10:C32:1560:GLN:OE1  | 10:C32:1601:TYR:CE1 | 2.35                     | 0.79              |
| 7:Q:166:GLU:OE2      | 7:Q:169:ARG:NH2     | 2.16                     | 0.79              |
| 5:P8:614:VAL:CB      | 5:P8:629:ARG:NH2    | 2.45                     | 0.79              |
| 10:C16:64:LEU:HD12   | 10:C16:70:ILE:HD12  | 1.63                     | 0.79              |
| 10:C16:1272:GLN:CD   | 10:C16:1289:LYS:HD2 | 2.08                     | 0.79              |
| 10:C16:1466:ARG:NH1  | 11:A24:127:SER:OG   | 2.16                     | 0.79              |
| 10:C16:1618:SER:O    | 10:C16:1620:ILE:N   | 2.15                     | 0.79              |
| 10:C24:1335:ILE:O    | 10:C24:1337:LEU:N   | 2.16                     | 0.79              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:V:730:GLN:N       | 13:V:731:PRO:HD2     | 1.95                     | 0.79              |
| 10:C:1618:SER:O      | 10:C:1620:ILE:N      | 2.15                     | 0.79              |
| 10:C8:1265:ARG:NH2   | 16:A8:115:SER:OG     | 2.16                     | 0.79              |
| 10:C8:1272:GLN:CD    | 10:C8:1289:LYS:HD2   | 2.08                     | 0.79              |
| 11:A16:312:LEU:CD1   | 11:A16:364:ILE:HD11  | 2.12                     | 0.79              |
| 11:A32:557:LEU:CD2   | 11:A32:561:ASP:HB3   | 2.12                     | 0.79              |
| 18:B:1279:THR:OG1    | 18:B:1289:ASP:OD1    | 1.99                     | 0.79              |
| 19:4:126:ARG:HH12    | 19:4:134:LYS:C       | 1.91                     | 0.79              |
| 21:H8:322:LEU:HD22   | 22:I8:300:LEU:CG     | 2.13                     | 0.79              |
| 21:H24:247:GLU:OE2   | 22:I24:181:LEU:HD23  | 1.80                     | 0.79              |
| 22:I24:131:ARG:NE    | 23:J24:557:ARG:NH2   | 2.31                     | 0.79              |
| 10:C32:386:ASN:O     | 10:C32:390:HIS:CD2   | 2.35                     | 0.79              |
| 10:C32:837:ARG:NH2   | 10:C32:890:ASP:HB3   | 1.98                     | 0.79              |
| 5:P:497:LEU:HA       | 6:O:290:MET:HE1      | 1.63                     | 0.79              |
| 5:P8:497:LEU:HA      | 6:O8:290:MET:HE1     | 1.63                     | 0.79              |
| 6:O16:28:SER:OG      | 6:O16:30:ASN:OD1     | 1.99                     | 0.79              |
| 10:C16:1034:SER:N    | 10:C16:1218:ARG:HH22 | 1.81                     | 0.79              |
| 10:C16:1250:ALA:HB2  | 10:C16:1309:ARG:HH12 | 1.47                     | 0.79              |
| 10:C:663:ILE:CG2     | 10:C:667:ILE:CD1     | 2.61                     | 0.79              |
| 10:C8:75:GLN:HE21    | 10:C8:112:PRO:HG3    | 1.46                     | 0.79              |
| 18:B:856:LEU:HD11    | 18:B:907:SER:HB2     | 1.64                     | 0.79              |
| 18:B:1045:LYS:HZ3    | 18:B:1100:LEU:HD23   | 1.47                     | 0.79              |
| 18:B:1164:GLU:OE1    | 18:B:1399:ILE:CG2    | 2.31                     | 0.79              |
| 18:B:1803:THR:C      | 18:B:1805:GLU:N      | 2.41                     | 0.79              |
| 21:H24:244:ARG:HH21  | 22:I24:177:VAL:HG13  | 1.47                     | 0.79              |
| 1:R:1078:SER:CB      | 5:P:713:LEU:CD2      | 2.61                     | 0.79              |
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:CB     | 2.31                     | 0.79              |
| 1:R8:1460:MET:HE3    | 1:R8:1463:GLN:OE1    | 1.81                     | 0.79              |
| 5:P8:105:ARG:HH22    | 5:P8:133:TYR:HB3     | 1.48                     | 0.79              |
| 7:Q16:219:GLY:HA2    | 7:Q16:221:TRP:NE1    | 1.98                     | 0.79              |
| 8:L8:1064:ASP:OD2    | 9:K8:1101:GLU:CD     | 2.26                     | 0.79              |
| 9:K:751:LEU:HD22     | 9:K:754:ARG:HH11     | 1.47                     | 0.79              |
| 10:C16:663:ILE:CG2   | 10:C16:667:ILE:CD1   | 2.61                     | 0.79              |
| 10:C16:1283:LEU:HD23 | 10:C16:1287:MET:HG3  | 1.64                     | 0.79              |
| 10:C24:663:ILE:CG2   | 10:C24:667:ILE:CD1   | 2.61                     | 0.79              |
| 12:A:557:LEU:CD2     | 12:A:561:ASP:HB3     | 2.12                     | 0.79              |
| 10:C:453:LEU:CB      | 10:C:486:LEU:CD2     | 2.61                     | 0.79              |
| 10:C:702:LEU:O       | 10:C:794:LYS:NZ      | 2.16                     | 0.79              |
| 18:B8:846:SER:HG     | 18:B8:899:LYS:HZ3    | 1.30                     | 0.79              |
| 19:48:126:ARG:HH12   | 19:48:134:LYS:C      | 1.91                     | 0.79              |
| 22:I8:131:ARG:NE     | 23:J8:557:ARG:NH2    | 2.31                     | 0.79              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 22:I24:155:PHE:CE1  | 22:I24:159:ARG:HD2  | 2.17                     | 0.79              |
| 23:J16:686:MET:HE1  | 23:J16:694:ARG:HH21 | 1.43                     | 0.79              |
| 12:A48:557:LEU:CD2  | 12:A48:561:ASP:HB3  | 2.12                     | 0.79              |
| 1:R:1424:LYS:HZ2    | 6:O:105:ASN:HD21    | 0.81                     | 0.79              |
| 3:N:263:TRP:HE1     | 3:N:279:GLY:HA2     | 1.46                     | 0.79              |
| 9:K8:695:GLU:OE1    | 9:K8:820:TYR:OH     | 2.00                     | 0.79              |
| 10:C16:453:LEU:CB   | 10:C16:486:LEU:CD2  | 2.61                     | 0.79              |
| 10:C16:837:ARG:NH2  | 10:C16:890:ASP:HB3  | 1.98                     | 0.79              |
| 10:C16:1560:GLN:OE1 | 10:C16:1601:TYR:CE1 | 2.35                     | 0.79              |
| 11:A24:557:LEU:CD2  | 11:A24:561:ASP:HB3  | 2.12                     | 0.79              |
| 10:C24:407:LYS:CE   | 10:C24:465:PHE:HE2  | 1.93                     | 0.79              |
| 10:C24:1547:LYS:HZ3 | 24:D24:1405:GLY:CA  | 1.96                     | 0.79              |
| 11:A40:103:GLU:CD   | 21:H16:323:TYR:CZ   | 2.61                     | 0.79              |
| 14:W:714:LEU:O      | 10:C8:1568:ARG:NH1  | 2.16                     | 0.79              |
| 10:C:75:GLN:NE2     | 10:C:112:PRO:HG3    | 1.98                     | 0.79              |
| 10:C:278:ARG:NH1    | 10:C:327:ILE:HG23   | 1.98                     | 0.79              |
| 10:C8:1163:LEU:CD2  | 10:C8:1166:SER:OG   | 2.29                     | 0.79              |
| 10:C8:1466:ARG:NH1  | 16:A8:127:SER:OG    | 2.16                     | 0.79              |
| 18:B:771:MET:HE3    | 18:B:840:VAL:CG1    | 2.12                     | 0.79              |
| 18:B8:968:PHE:CB    | 18:B8:1040:MET:CE   | 2.60                     | 0.79              |
| 21:H8:244:ARG:HH21  | 22:I8:177:VAL:HG13  | 1.47                     | 0.79              |
| 22:I16:131:ARG:NE   | 23:J16:557:ARG:NH2  | 2.31                     | 0.79              |
| 10:C32:390:HIS:CG   | 10:C32:452:LEU:CB   | 2.65                     | 0.79              |
| 10:C32:761:VAL:HG21 | 10:C32:826:TYR:HA   | 1.65                     | 0.79              |
| 1:R:979:GLN:HB2     | 24:D:1438:ALA:CB    | 2.13                     | 0.79              |
| 2:M:552:PHE:HZ      | 2:M:559:PHE:HE2     | 1.28                     | 0.79              |
| 2:M8:377:ARG:CZ     | 2:M8:477:ASP:HB3    | 2.12                     | 0.79              |
| 6:O8:180:GLY:C      | 6:O8:182:GLU:H      | 1.90                     | 0.79              |
| 7:Q8:219:GLY:HA2    | 7:Q8:221:TRP:NE1    | 1.98                     | 0.79              |
| 7:Q16:295:SER:C     | 7:Q16:297:VAL:H     | 1.91                     | 0.79              |
| 9:K8:614:PHE:C      | 9:K8:683:GLN:HE22   | 1.91                     | 0.79              |
| 10:C16:453:LEU:CD2  | 10:C16:459:LEU:HD11 | 2.08                     | 0.79              |
| 10:C16:1814:LYS:HE2 | 23:J32:738:MET:SD   | 2.22                     | 0.79              |
| 10:C24:1703:ILE:CD1 | 10:C24:1741:MET:CE  | 2.61                     | 0.79              |
| 12:A:312:LEU:CD1    | 12:A:364:ILE:HD11   | 2.12                     | 0.79              |
| 13:V:783:TRP:HZ2    | 14:W:671:GLU:HG3    | 1.49                     | 0.79              |
| 10:C8:453:LEU:CB    | 10:C8:486:LEU:CD2   | 2.61                     | 0.79              |
| 11:A16:212:LYS:HE2  | 11:A16:585:MET:HE1  | 0.80                     | 0.79              |
| 11:A16:703:ALA:O    | 24:D16:1398:ARG:NH1 | 2.16                     | 0.79              |
| 18:B:719:GLU:OE2    | 18:B:766:LYS:NZ     | 2.15                     | 0.79              |
| 20:E8:49:THR:HG23   | 20:E8:121:VAL:CG1   | 2.11                     | 0.79              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 24:D16:342:LEU:HD11  | 24:D16:348:MET:HE3  | 1.63                     | 0.79              |
| 24:D40:749:ARG:NH1   | 24:D40:963:GLN:O    | 2.16                     | 0.79              |
| 1:R:1165:MET:HE3     | 1:R:1220:GLN:CG     | 2.14                     | 0.78              |
| 1:R:1212:SER:OG      | 1:R:1218:LYS:NZ     | 2.15                     | 0.78              |
| 1:R8:1212:SER:OG     | 1:R8:1218:LYS:NZ    | 2.15                     | 0.78              |
| 1:R16:1460:MET:HE3   | 1:R16:1463:GLN:OE1  | 1.81                     | 0.78              |
| 6:O:28:SER:OG        | 6:O:30:ASN:OD1      | 1.99                     | 0.78              |
| 6:O:82:LEU:CD2       | 6:O:103:MET:CE      | 2.59                     | 0.78              |
| 6:O:164:GLY:O        | 6:O:166:PRO:HD3     | 1.82                     | 0.78              |
| 8:L:601:HIS:HE1      | 8:L:631:LEU:HD22    | 0.97                     | 0.78              |
| 9:K8:847:LEU:HD23    | 9:K8:910:SER:OG     | 1.83                     | 0.78              |
| 10:C16:1624:LEU:HD23 | 10:C16:1628:SER:HB2 | 1.64                     | 0.78              |
| 10:C24:390:HIS:CG    | 10:C24:452:LEU:CB   | 2.66                     | 0.78              |
| 10:C24:764:ILE:HD12  | 10:C24:781:VAL:HG21 | 1.66                     | 0.78              |
| 10:C24:837:ARG:NH2   | 10:C24:890:ASP:HB3  | 1.98                     | 0.78              |
| 12:A:440:LEU:HB3     | 12:A:443:LEU:HD12   | 1.57                     | 0.78              |
| 18:B:1768:ILE:CG2    | 18:B:1770:THR:HG22  | 2.09                     | 0.78              |
| 18:B8:1101:TYR:CE1   | 18:B8:1105:LEU:HD11 | 2.17                     | 0.78              |
| 19:4:189:LEU:CD2     | 19:4:203:LEU:HD23   | 2.13                     | 0.78              |
| 23:J8:686:MET:HE1    | 23:J8:694:ARG:HH21  | 1.43                     | 0.78              |
| 21:H16:322:LEU:HD22  | 22:I16:300:LEU:CG   | 2.13                     | 0.78              |
| 2:M:847:PHE:CB       | 4:T:656:TRP:CH2     | 2.45                     | 0.78              |
| 3:N:19:MET:HE2       | 3:N:23:GLY:HA2      | 1.65                     | 0.78              |
| 1:R8:1078:SER:HB2    | 5:P8:713:LEU:HD21   | 1.65                     | 0.78              |
| 1:R16:1381:GLU:O     | 1:R16:1382:LYS:HG3  | 1.82                     | 0.78              |
| 5:P16:394:ASN:C      | 5:P16:396:SER:H     | 1.90                     | 0.78              |
| 6:O16:180:GLY:C      | 6:O16:182:GLU:H     | 1.90                     | 0.78              |
| 7:Q16:27:GLN:HE22    | 7:Q16:33:ARG:HG2    | 1.45                     | 0.78              |
| 10:C16:1265:ARG:NH2  | 11:A24:115:SER:OG   | 2.16                     | 0.78              |
| 10:C16:1626:GLN:HE21 | 10:C16:1692:LYS:HZ3 | 1.27                     | 0.78              |
| 10:C16:1703:ILE:CD1  | 10:C16:1741:MET:CE  | 2.61                     | 0.78              |
| 10:C24:702:LEU:O     | 10:C24:794:LYS:NZ   | 2.15                     | 0.78              |
| 10:C24:1560:GLN:OE1  | 10:C24:1601:TYR:CE1 | 2.35                     | 0.78              |
| 14:W:746:THR:CG2     | 15:J:675:ASN:HD21   | 1.96                     | 0.78              |
| 10:C8:702:LEU:O      | 10:C8:794:LYS:NZ    | 2.16                     | 0.78              |
| 10:C8:1703:ILE:CD1   | 10:C8:1741:MET:CE   | 2.61                     | 0.78              |
| 17:F:74:ILE:CG2      | 17:F:76:ASP:HB2     | 2.13                     | 0.78              |
| 18:B8:789:LEU:HD23   | 18:B8:793:LEU:CD1   | 2.12                     | 0.78              |
| 10:C32:1618:SER:O    | 10:C32:1620:ILE:N   | 2.15                     | 0.78              |
| 10:C32:1703:ILE:CD1  | 10:C32:1741:MET:CE  | 2.61                     | 0.78              |
| 3:N:116:ILE:CG2      | 3:N:177:TYR:CE1     | 2.67                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:R8:1165:MET:HE3   | 1:R8:1220:GLN:CG    | 2.14                     | 0.78              |
| 6:O:282:GLU:HB2     | 6:O:284:TRP:CZ2     | 2.19                     | 0.78              |
| 7:Q8:166:GLU:OE2    | 7:Q8:169:ARG:NH2    | 2.16                     | 0.78              |
| 7:Q16:166:GLU:OE2   | 7:Q16:169:ARG:NH2   | 2.16                     | 0.78              |
| 9:K8:751:LEU:HD22   | 9:K8:754:ARG:HH11   | 1.46                     | 0.78              |
| 9:K8:792:LEU:HD23   | 9:K8:864:ILE:CD1    | 2.13                     | 0.78              |
| 10:C16:565:ARG:HH22 | 10:C16:569:PHE:HD2  | 1.28                     | 0.78              |
| 10:C16:761:VAL:HG21 | 10:C16:826:TYR:HA   | 1.65                     | 0.78              |
| 10:C8:556:VAL:HG13  | 10:C8:565:ARG:NH2   | 1.94                     | 0.78              |
| 11:A32:112:ALA:CB   | 18:B8:1416:LYS:NZ   | 2.46                     | 0.78              |
| 11:A32:706:SER:HB2  | 24:D32:1398:ARG:HD3 | 1.65                     | 0.78              |
| 17:F24:74:ILE:CG2   | 17:F24:76:ASP:HB2   | 2.13                     | 0.78              |
| 18:B:968:PHE:CB     | 18:B:1040:MET:CE    | 2.60                     | 0.78              |
| 18:B:1505:MET:CE    | 18:B:1518:VAL:HG21  | 2.13                     | 0.78              |
| 18:B8:583:ARG:NH1   | 18:B8:711:CYS:CB    | 2.43                     | 0.78              |
| 18:B8:771:MET:HE3   | 18:B8:840:VAL:CG1   | 2.12                     | 0.78              |
| 24:D8:342:LEU:HD11  | 24:D8:348:MET:HE3   | 1.63                     | 0.78              |
| 10:C32:278:ARG:NH1  | 10:C32:327:ILE:HG23 | 1.98                     | 0.78              |
| 10:C32:407:LYS:HZ2  | 10:C32:465:PHE:HE2  | 1.27                     | 0.78              |
| 5:P:394:ASN:C       | 5:P:396:SER:H       | 1.90                     | 0.78              |
| 6:O8:282:GLU:HB2    | 6:O8:284:TRP:CZ2    | 2.19                     | 0.78              |
| 5:P16:592:SER:C     | 5:P16:594:ILE:H     | 1.90                     | 0.78              |
| 6:O16:282:GLU:HB2   | 6:O16:284:TRP:CZ2   | 2.19                     | 0.78              |
| 9:K8:1048:GLN:HG3   | 9:K8:1074:ARG:HH22  | 1.47                     | 0.78              |
| 10:C16:1541:PHE:CE1 | 10:C16:1649:LYS:HD2 | 2.19                     | 0.78              |
| 10:C16:1622:SER:OG  | 10:C16:1623:ILE:N   | 2.08                     | 0.78              |
| 10:C24:627:VAL:CG1  | 10:C24:628:GLY:H    | 1.95                     | 0.78              |
| 10:C:1335:ILE:O     | 10:C:1337:LEU:N     | 2.16                     | 0.78              |
| 11:A16:112:ALA:CB   | 18:B:1416:LYS:NZ    | 2.46                     | 0.78              |
| 11:A16:676:TYR:OH   | 24:D16:1394:SER:C   | 2.27                     | 0.78              |
| 18:B8:1505:MET:CE   | 18:B8:1518:VAL:HG21 | 2.12                     | 0.78              |
| 21:H:244:ARG:HH21   | 22:I:177:VAL:HG13   | 1.47                     | 0.78              |
| 23:J32:686:MET:HE1  | 23:J32:694:ARG:HH21 | 1.43                     | 0.78              |
| 10:C32:110:ARG:HH12 | 10:C32:118:LEU:HD11 | 1.41                     | 0.78              |
| 1:R:979:GLN:CD      | 24:D:1438:ALA:H     | 1.91                     | 0.78              |
| 1:R8:1266:THR:CA    | 5:P8:684:ARG:HH22   | 1.94                     | 0.78              |
| 1:R16:1442:THR:HG21 | 3:N16:13:ILE:HD12   | 1.63                     | 0.78              |
| 5:P16:112:LEU:HD21  | 5:P16:122:TYR:CE2   | 2.18                     | 0.78              |
| 9:K:786:GLN:HE22    | 9:K:794:ARG:NH1     | 1.81                     | 0.78              |
| 10:C16:345:MET:HE3  | 10:C16:401:ILE:HD13 | 1.49                     | 0.78              |
| 10:C16:1688:ARG:HG2 | 23:J32:735:LYS:HE3  | 1.64                     | 0.78              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1272:GLN:CD  | 10:C24:1289:LYS:HD2  | 2.08                     | 0.78              |
| 13:V:847:ASN:ND2    | 14:W:723:TYR:HE1     | 1.82                     | 0.78              |
| 14:W:585:ILE:HD12   | 15:J:576:LEU:HD12    | 1.64                     | 0.78              |
| 10:C:1619:PRO:C     | 10:C:1621:LYS:H      | 1.89                     | 0.78              |
| 10:C8:1250:ALA:HB2  | 10:C8:1309:ARG:HH12  | 1.47                     | 0.78              |
| 10:C8:1283:LEU:HD23 | 10:C8:1287:MET:HG3   | 1.65                     | 0.78              |
| 11:A16:711:ARG:HD3  | 24:D16:1398:ARG:CG   | 2.14                     | 0.78              |
| 11:A32:91:GLU:HB2   | 18:B8:1112:LYS:HZ3   | 0.89                     | 0.78              |
| 18:B8:90:ILE:HD12   | 18:B8:105:VAL:CG2    | 2.14                     | 0.78              |
| 18:B8:1768:ILE:CG2  | 18:B8:1770:THR:HG22  | 2.09                     | 0.78              |
| 18:B8:1803:THR:C    | 18:B8:1805:GLU:H     | 1.91                     | 0.78              |
| 24:D:342:LEU:HD11   | 24:D:348:MET:HE3     | 1.63                     | 0.78              |
| 24:D32:342:LEU:HD11 | 24:D32:348:MET:HE3   | 1.63                     | 0.78              |
| 24:D32:749:ARG:HH22 | 24:D40:397:ALA:H     | 0.84                     | 0.78              |
| 12:A48:212:LYS:HE2  | 12:A48:585:MET:HE1   | 0.80                     | 0.78              |
| 2:M:762:LEU:CB      | 2:M:813:ASN:HD21     | 1.85                     | 0.78              |
| 2:M8:540:TYR:CD1    | 2:M8:555:LEU:CD2     | 2.67                     | 0.78              |
| 7:Q:219:GLY:HA2     | 7:Q:221:TRP:NE1      | 1.98                     | 0.78              |
| 5:P8:158:VAL:CG1    | 5:P8:248:ILE:HG23    | 2.13                     | 0.78              |
| 5:P16:112:LEU:HD22  | 5:P16:122:TYR:CG     | 2.11                     | 0.78              |
| 10:C16:1271:PHE:CZ  | 10:C16:1284:ASP:OD1  | 2.29                     | 0.78              |
| 10:C8:1335:ILE:O    | 10:C8:1337:LEU:N     | 2.16                     | 0.78              |
| 11:A16:246:SER:OG   | 11:A16:500:ASP:OD2   | 2.02                     | 0.78              |
| 18:B8:1164:GLU:OE1  | 18:B8:1399:ILE:CG2   | 2.31                     | 0.78              |
| 18:B8:1210:CYS:HG   | 18:B8:1234:MET:CE    | 1.80                     | 0.78              |
| 19:4:250:ILE:CB     | 20:E:165:ARG:HH22    | 1.95                     | 0.78              |
| 20:E:429:PRO:CB     | 24:D:69:VAL:HG22     | 2.14                     | 0.78              |
| 21:H24:322:LEU:HD22 | 22:I24:300:LEU:CG    | 2.13                     | 0.78              |
| 24:D32:1109:LEU:CD2 | 24:D32:1156:SER:HB2  | 2.14                     | 0.78              |
| 10:C32:1010:ALA:N   | 10:C32:1192:ARG:HH21 | 1.81                     | 0.78              |
| 1:R8:1075:LYS:HE2   | 5:P8:713:LEU:O       | 1.83                     | 0.78              |
| 2:M8:351:ALA:HB1    | 8:L8:219:ILE:HG22    | 1.61                     | 0.78              |
| 2:M8:625:HIS:HA     | 3:N8:165:GLY:CA      | 2.10                     | 0.78              |
| 5:P:401:ARG:HH21    | 5:P:404:ILE:CG2      | 1.93                     | 0.78              |
| 7:Q:125:TYR:CD1     | 7:Q:167:GLY:HA2      | 2.19                     | 0.78              |
| 5:P8:73:ASN:HB2     | 6:O8:5:MET:SD        | 2.24                     | 0.78              |
| 7:Q16:125:TYR:CD1   | 7:Q16:167:GLY:HA2    | 2.19                     | 0.78              |
| 9:K:1049:ASP:O      | 9:K:1050:GLU:C       | 2.13                     | 0.78              |
| 9:K8:792:LEU:CD2    | 9:K8:864:ILE:CD1     | 2.62                     | 0.78              |
| 10:C16:278:ARG:NH1  | 10:C16:327:ILE:HG23  | 1.98                     | 0.78              |
| 10:C24:453:LEU:CD2  | 10:C24:459:LEU:HD11  | 2.08                     | 0.78              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:453:LEU:CB   | 10:C24:486:LEU:CD2   | 2.61                     | 0.78              |
| 10:C24:1265:ARG:NH2 | 11:A40:115:SER:OG    | 2.16                     | 0.78              |
| 10:C24:1618:SER:O   | 10:C24:1620:ILE:N    | 2.15                     | 0.78              |
| 12:A:127:SER:OG     | 10:C:1466:ARG:NH1    | 2.16                     | 0.78              |
| 10:C:1272:GLN:CD    | 10:C:1289:LYS:HD2    | 2.08                     | 0.78              |
| 10:C8:278:ARG:NH1   | 10:C8:327:ILE:HG23   | 1.98                     | 0.78              |
| 11:A16:148:LEU:CD1  | 18:B:1956:ILE:CD1    | 2.61                     | 0.78              |
| 11:A32:212:LYS:HE3  | 11:A32:585:MET:SD    | 2.24                     | 0.78              |
| 18:B:90:ILE:HD12    | 18:B:105:VAL:CG2     | 2.14                     | 0.78              |
| 18:B:603:PHE:HB2    | 18:B:619:ARG:CZ      | 2.13                     | 0.78              |
| 10:C32:75:GLN:NE2   | 10:C32:112:PRO:HG3   | 1.98                     | 0.78              |
| 2:M16:625:HIS:HA    | 3:N16:165:GLY:CA     | 2.10                     | 0.78              |
| 5:P:220:GLU:OE2     | 5:P:232:ARG:CZ       | 2.32                     | 0.78              |
| 5:P:592:SER:C       | 5:P:594:ILE:H        | 1.90                     | 0.78              |
| 7:Q:295:SER:C       | 7:Q:297:VAL:H        | 1.91                     | 0.78              |
| 9:K16:894:LYS:HZ1   | 9:K16:1057:GLU:HB3   | 1.48                     | 0.78              |
| 10:C16:1424:GLN:NE2 | 10:C16:1478:VAL:HG11 | 1.99                     | 0.78              |
| 10:C24:75:GLN:NE2   | 10:C24:112:PRO:HG3   | 1.98                     | 0.78              |
| 10:C24:1126:ASP:OD2 | 24:D24:1069:GLY:HA3  | 1.82                     | 0.78              |
| 10:C24:1424:GLN:NE2 | 10:C24:1478:VAL:HG11 | 1.99                     | 0.78              |
| 12:A:115:SER:OG     | 10:C:1265:ARG:NH2    | 2.16                     | 0.78              |
| 13:V:902:MET:HG3    | 15:J:696:LEU:HD21    | 1.66                     | 0.78              |
| 14:W:517:GLU:N      | 14:W:605:ASN:N       | 2.32                     | 0.78              |
| 14:W:598:ILE:HG23   | 14:W:626:LEU:CD2     | 2.14                     | 0.78              |
| 10:C:764:ILE:HD12   | 10:C:781:VAL:HG21    | 1.66                     | 0.78              |
| 10:C:837:ARG:NH2    | 10:C:890:ASP:HB3     | 1.98                     | 0.78              |
| 10:C:1034:SER:N     | 10:C:1218:ARG:HH22   | 1.81                     | 0.78              |
| 11:A32:112:ALA:HB1  | 18:B8:1416:LYS:HZ1   | 1.44                     | 0.78              |
| 18:B8:603:PHE:HB2   | 18:B8:619:ARG:CZ     | 2.13                     | 0.78              |
| 18:B8:1668:PHE:CZ   | 18:B8:1731:PHE:CD2   | 2.72                     | 0.78              |
| 21:H8:204:LEU:HD21  | 22:I8:140:CYS:SG     | 2.24                     | 0.78              |
| 2:M16:225:ASP:CB    | 2:M16:606:GLN:NE2    | 2.47                     | 0.78              |
| 5:P:11:GLY:N        | 5:P:26:TYR:OH        | 2.17                     | 0.78              |
| 5:P8:291:LEU:HD12   | 5:P8:299:CYS:SG      | 2.24                     | 0.78              |
| 10:C16:453:LEU:HD22 | 10:C16:459:LEU:HD22  | 1.60                     | 0.78              |
| 10:C16:702:LEU:O    | 10:C16:794:LYS:NZ    | 2.15                     | 0.78              |
| 10:C24:1074:LEU:CG  | 18:B8:256:VAL:O      | 2.31                     | 0.78              |
| 11:A32:148:LEU:CD1  | 18:B8:1956:ILE:CD1   | 2.61                     | 0.78              |
| 18:B:1668:PHE:CZ    | 18:B:1731:PHE:CD2    | 2.72                     | 0.78              |
| 18:B8:690:TRP:CZ3   | 18:B8:739:VAL:HG21   | 2.19                     | 0.78              |
| 18:B8:842:ASN:O     | 18:B8:899:LYS:NZ     | 2.17                     | 0.78              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B8:1130:LEU:CD2  | 18:B8:1132:TRP:NE1   | 2.45                     | 0.78              |
| 21:H24:204:LEU:HD21 | 22:I24:140:CYS:SG    | 2.24                     | 0.78              |
| 2:M:225:ASP:CB      | 2:M:606:GLN:NE2      | 2.47                     | 0.78              |
| 3:N8:19:MET:HE2     | 3:N8:23:GLY:HA2      | 1.65                     | 0.78              |
| 3:N8:116:ILE:CG2    | 3:N8:177:TYR:CE1     | 2.67                     | 0.78              |
| 1:R16:1165:MET:HE3  | 1:R16:1220:GLN:CG    | 2.14                     | 0.78              |
| 2:M16:217:ILE:HD11  | 3:N16:28:THR:HG21    | 1.66                     | 0.78              |
| 8:L8:608:PHE:CE2    | 8:L8:635:MET:CB      | 2.66                     | 0.78              |
| 8:L8:1041:SER:CB    | 8:L8:1054:HIS:HE1    | 1.92                     | 0.78              |
| 9:K8:786:GLN:HE22   | 9:K8:794:ARG:NH1     | 1.81                     | 0.78              |
| 10:C16:390:HIS:HD2  | 10:C16:452:LEU:CD2   | 1.97                     | 0.78              |
| 11:A24:212:LYS:CE   | 11:A24:585:MET:HE3   | 2.14                     | 0.78              |
| 10:C24:1034:SER:N   | 10:C24:1218:ARG:HH22 | 1.81                     | 0.78              |
| 14:W:739:ARG:NH2    | 15:J:664:GLN:NE2     | 2.32                     | 0.78              |
| 10:C8:837:ARG:NH2   | 10:C8:890:ASP:HB3    | 1.98                     | 0.78              |
| 10:C8:1034:SER:N    | 10:C8:1218:ARG:HH22  | 1.81                     | 0.78              |
| 10:C8:1541:PHE:CE1  | 10:C8:1649:LYS:HD2   | 2.19                     | 0.78              |
| 18:B:603:PHE:CB     | 18:B:619:ARG:CZ      | 2.62                     | 0.78              |
| 18:B8:603:PHE:CB    | 18:B8:619:ARG:CZ     | 2.62                     | 0.78              |
| 18:B8:771:MET:CE    | 18:B8:840:VAL:HG11   | 2.13                     | 0.78              |
| 19:4:100:ILE:CD1    | 19:4:274:PHE:HE1     | 1.97                     | 0.78              |
| 24:D32:1099:ARG:HG3 | 24:D32:1101:HIS:NE2  | 1.99                     | 0.78              |
| 10:C32:664:ASN:HA   | 10:C32:667:ILE:HG13  | 1.66                     | 0.78              |
| 10:C32:1424:GLN:NE2 | 10:C32:1478:VAL:HG11 | 1.99                     | 0.78              |
| 2:M8:225:ASP:HB3    | 2:M8:606:GLN:NE2     | 1.99                     | 0.77              |
| 2:M16:420:CYS:HB3   | 8:L16:391:TRP:CH2    | 2.19                     | 0.77              |
| 7:Q:244:ILE:HG23    | 7:Q:289:TYR:OH       | 1.85                     | 0.77              |
| 8:L:1074:ARG:HD2    | 9:K:1089:LYS:HB3     | 1.66                     | 0.77              |
| 9:K:1214:TYR:CB     | 9:K:1269:CYS:SG      | 2.71                     | 0.77              |
| 11:A24:54:ASN:HB3   | 11:A24:59:GLN:NE2    | 1.98                     | 0.77              |
| 10:C24:878:ARG:HH21 | 10:C24:885:VAL:HG23  | 1.49                     | 0.77              |
| 11:A40:212:LYS:HE3  | 11:A40:585:MET:SD    | 2.24                     | 0.77              |
| 10:C:65:PRO:CG      | 10:C:96:ARG:NH2      | 2.44                     | 0.77              |
| 10:C:761:VAL:HG21   | 10:C:826:TYR:HA      | 1.65                     | 0.77              |
| 10:C8:75:GLN:NE2    | 10:C8:112:PRO:HG3    | 1.98                     | 0.77              |
| 11:A32:90:PHE:CE1   | 18:B8:1788:ILE:HG23  | 2.11                     | 0.77              |
| 11:A32:91:GLU:CG    | 18:B8:1112:LYS:HZ3   | 1.97                     | 0.77              |
| 17:F16:74:ILE:CG2   | 17:F16:76:ASP:HB2    | 2.14                     | 0.77              |
| 19:4:109:GLN:O      | 19:4:418:LYS:CE      | 2.32                     | 0.77              |
| 22:I:290:ASP:OD1    | 22:I:293:LYS:HD2     | 1.85                     | 0.77              |
| 22:I8:171:MET:HE2   | 23:J8:592:VAL:HG13   | 1.65                     | 0.77              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:C32:453:LEU:CB   | 10:C32:486:LEU:CD2 | 2.61                     | 0.77              |
| 1:R:1266:THR:OG1    | 5:P:684:ARG:NH2    | 2.16                     | 0.77              |
| 2:M8:225:ASP:CB     | 2:M8:606:GLN:NE2   | 2.47                     | 0.77              |
| 2:M8:571:TYR:CD1    | 2:M8:595:LEU:HD12  | 2.19                     | 0.77              |
| 1:R16:634:ARG:HD3   | 4:T16:160:HIS:CE1  | 2.19                     | 0.77              |
| 1:R16:1101:ARG:NH1  | 1:R16:1188:TYR:CD2 | 2.53                     | 0.77              |
| 5:P16:291:LEU:HD12  | 5:P16:299:CYS:SG   | 2.24                     | 0.77              |
| 9:K:1048:GLN:CD     | 9:K:1128:ARG:HG2   | 2.09                     | 0.77              |
| 11:A24:1:MET:SD     | 22:I8:151:GLU:OE1  | 2.43                     | 0.77              |
| 12:A:207:TYR:HB3    | 12:A:536:HIS:NE2   | 1.99                     | 0.77              |
| 10:C:1549:VAL:HG13  | 10:C:1592:VAL:CG1  | 2.15                     | 0.77              |
| 10:C8:453:LEU:HB2   | 10:C8:486:LEU:HD23 | 1.67                     | 0.77              |
| 10:C8:798:VAL:HG11  | 10:C8:802:TRP:CH2  | 2.20                     | 0.77              |
| 11:A16:54:ASN:HB3   | 11:A16:59:GLN:NE2  | 1.98                     | 0.77              |
| 18:B:442:SER:O      | 18:B:449:ARG:NH2   | 2.16                     | 0.77              |
| 18:B8:1130:LEU:CD2  | 18:B8:1132:TRP:HE1 | 1.93                     | 0.77              |
| 19:48:183:ARG:NH1   | 19:48:245:GLY:CA   | 2.32                     | 0.77              |
| 21:H:204:LEU:HD21   | 22:I:140:CYS:SG    | 2.24                     | 0.77              |
| 21:H8:322:LEU:HD13  | 23:J8:689:LEU:CG   | 2.14                     | 0.77              |
| 10:C32:1265:ARG:NH2 | 12:A48:115:SER:OG  | 2.16                     | 0.77              |
| 2:M:202:LYS:HZ2     | 2:M:208:SER:C      | 1.86                     | 0.77              |
| 3:N:158:TRP:CD2     | 3:N:179:LEU:CD2    | 2.67                     | 0.77              |
| 7:Q:279:LEU:HD21    | 7:Q:315:GLY:HA3    | 1.66                     | 0.77              |
| 5:P8:592:SER:C      | 5:P8:594:ILE:H     | 1.90                     | 0.77              |
| 5:P16:220:GLU:OE2   | 5:P16:232:ARG:CZ   | 2.32                     | 0.77              |
| 9:K:840:TRP:HZ3     | 9:K:907:ILE:HD12   | 1.48                     | 0.77              |
| 9:K8:1198:LEU:HD12  | 9:K8:1267:LEU:HD22 | 1.64                     | 0.77              |
| 10:C16:1547:LYS:HE2 | 24:D8:1405:GLY:H   | 1.48                     | 0.77              |
| 11:A40:207:TYR:HB3  | 11:A40:536:HIS:NE2 | 2.00                     | 0.77              |
| 10:C:407:LYS:NZ     | 10:C:465:PHE:HE2   | 1.82                     | 0.77              |
| 10:C:1624:LEU:HD23  | 10:C:1628:SER:HB2  | 1.65                     | 0.77              |
| 10:C:1703:ILE:CD1   | 10:C:1741:MET:CE   | 2.61                     | 0.77              |
| 10:C8:1466:ARG:NH2  | 16:A8:124:ASN:HA   | 2.00                     | 0.77              |
| 18:B8:428:GLN:CG    | 18:B8:584:ARG:CZ   | 2.46                     | 0.77              |
| 21:H24:243:LEU:HD11 | 23:J24:603:LEU:HG  | 1.66                     | 0.77              |
| 2:M:217:ILE:HD11    | 3:N:28:THR:HG21    | 1.66                     | 0.77              |
| 5:P:158:VAL:CG1     | 5:P:248:ILE:HG23   | 2.13                     | 0.77              |
| 5:P:401:ARG:HD2     | 5:P:414:VAL:CG1    | 2.15                     | 0.77              |
| 5:P8:11:GLY:N       | 5:P8:26:TYR:OH     | 2.17                     | 0.77              |
| 9:K:847:LEU:HD23    | 9:K:910:SER:OG     | 1.83                     | 0.77              |
| 9:K:923:ILE:HG22    | 9:K:929:ARG:HE     | 1.50                     | 0.77              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A24:747:MET:CE    | 24:D16:167:ARG:HH12 | 1.97                     | 0.77              |
| 11:A40:207:TYR:HB3   | 11:A40:536:HIS:CD2  | 2.20                     | 0.77              |
| 17:F8:74:ILE:C       | 17:F8:76:ASP:N      | 2.38                     | 0.77              |
| 11:A32:1:MET:SD      | 22:I24:151:GLU:OE1  | 2.43                     | 0.77              |
| 18:B8:442:SER:O      | 18:B8:449:ARG:NH2   | 2.16                     | 0.77              |
| 18:B8:1940:ALA:HB3   | 18:B8:1950:ILE:CD1  | 2.14                     | 0.77              |
| 20:E8:353:ILE:CB     | 20:E8:413:PHE:CE2   | 2.67                     | 0.77              |
| 22:I:268:ARG:HG2     | 22:I:272:TYR:CE2    | 2.19                     | 0.77              |
| 22:I16:199:PHE:HB3   | 23:J16:620:MET:SD   | 2.25                     | 0.77              |
| 22:I16:290:ASP:OD1   | 22:I16:293:LYS:HD2  | 1.85                     | 0.77              |
| 24:D:405:GLN:HG2     | 24:D16:10:ARG:HH11  | 1.04                     | 0.77              |
| 10:C32:702:LEU:O     | 10:C32:794:LYS:NZ   | 2.15                     | 0.77              |
| 10:C32:1549:VAL:HG13 | 10:C32:1592:VAL:CG1 | 2.14                     | 0.77              |
| 1:R:1168:LEU:HD23    | 1:R:1216:ILE:HG13   | 1.66                     | 0.77              |
| 2:M:250:LEU:HD13     | 2:M:286:SER:HB3     | 1.67                     | 0.77              |
| 3:N16:158:TRP:CD2    | 3:N16:179:LEU:CD2   | 2.67                     | 0.77              |
| 5:P8:220:GLU:OE2     | 5:P8:232:ARG:CZ     | 2.32                     | 0.77              |
| 8:L16:856:LEU:HA     | 9:K16:1281:SER:OG   | 1.85                     | 0.77              |
| 9:K8:923:ILE:HG22    | 9:K8:929:ARG:HE     | 1.50                     | 0.77              |
| 9:K8:1142:ARG:HH21   | 9:K8:1204:THR:HA    | 1.48                     | 0.77              |
| 10:C24:407:LYS:HZ2   | 10:C24:465:PHE:HE2  | 1.33                     | 0.77              |
| 11:A32:54:ASN:HB3    | 11:A32:59:GLN:NE2   | 1.98                     | 0.77              |
| 11:A32:207:TYR:HB3   | 11:A32:536:HIS:CD2  | 2.20                     | 0.77              |
| 18:B:1803:THR:C      | 18:B:1805:GLU:H     | 1.91                     | 0.77              |
| 19:4:251:ARG:HH21    | 19:4:254:LEU:HD23   | 1.50                     | 0.77              |
| 21:H:243:LEU:HD11    | 23:J32:603:LEU:HG   | 1.66                     | 0.77              |
| 21:H:322:LEU:HD22    | 22:I:300:LEU:CG     | 2.13                     | 0.77              |
| 21:H16:204:LEU:HD21  | 22:I16:140:CYS:SG   | 2.24                     | 0.77              |
| 12:A48:557:LEU:HD22  | 12:A48:561:ASP:HB3  | 1.67                     | 0.77              |
| 1:R:1059:ILE:HG23    | 24:D:1448:TYR:OH    | 1.85                     | 0.77              |
| 2:M8:593:HIS:HD2     | 3:N8:224:LEU:HD22   | 1.49                     | 0.77              |
| 2:M8:669:ALA:HB2     | 2:M8:684:GLN:HE21   | 1.46                     | 0.77              |
| 5:P:600:PHE:CG       | 5:P:638:SER:HB2     | 2.19                     | 0.77              |
| 9:K:1019:ARG:HD3     | 9:K:1059:ARG:CD     | 2.14                     | 0.77              |
| 9:K:1142:ARG:HH21    | 9:K:1204:THR:CA     | 1.98                     | 0.77              |
| 9:K:1198:LEU:HD12    | 9:K:1267:LEU:HD22   | 1.64                     | 0.77              |
| 9:K:1214:TYR:OH      | 9:K:1230:LEU:O      | 2.03                     | 0.77              |
| 10:C16:75:GLN:NE2    | 10:C16:112:PRO:HG3  | 1.98                     | 0.77              |
| 10:C16:627:VAL:CG1   | 10:C16:628:GLY:H    | 1.95                     | 0.77              |
| 10:C24:761:VAL:HG21  | 10:C24:826:TYR:HA   | 1.65                     | 0.77              |
| 10:C24:1541:PHE:CE1  | 10:C24:1649:LYS:HD2 | 2.18                     | 0.77              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A40:156:MET:HG2  | 11:A40:555:HIS:NE2  | 1.44                     | 0.77              |
| 11:A40:246:SER:OG   | 11:A40:500:ASP:OD2  | 2.02                     | 0.77              |
| 10:C:1250:ALA:CB    | 10:C:1309:ARG:NH1   | 2.48                     | 0.77              |
| 10:C8:65:PRO:CG     | 10:C8:96:ARG:NH2    | 2.44                     | 0.77              |
| 11:A16:629:LEU:C    | 11:A16:678:LYS:HZ3  | 1.91                     | 0.77              |
| 17:F8:74:ILE:CG2    | 17:F8:76:ASP:HB2    | 2.14                     | 0.77              |
| 11:A32:246:SER:OG   | 11:A32:500:ASP:OD2  | 2.02                     | 0.77              |
| 18:B8:13:TRP:HB3    | 18:B8:46:TRP:CZ2    | 2.20                     | 0.77              |
| 22:I:171:MET:HE2    | 23:J32:592:VAL:HG13 | 1.65                     | 0.77              |
| 24:D40:1105:ALA:HB2 | 24:D40:1134:GLN:NE2 | 1.99                     | 0.77              |
| 10:C32:1466:ARG:NH2 | 12:A48:124:ASN:HA   | 2.00                     | 0.77              |
| 1:R:1033:LYS:HG2    | 24:D:1436:ARG:HE    | 1.47                     | 0.77              |
| 2:M:246:ALA:HB3     | 2:M:247:PRO:HD3     | 1.67                     | 0.77              |
| 2:M:403:LEU:HD21    | 2:M:425:ALA:HB3     | 1.67                     | 0.77              |
| 1:R8:1191:LYS:HB2   | 24:D40:1453:GLU:HG2 | 1.66                     | 0.77              |
| 2:M8:202:LYS:HZ1    | 2:M8:207:SER:C      | 1.93                     | 0.77              |
| 3:N16:116:ILE:CG2   | 3:N16:177:TYR:CE1   | 2.67                     | 0.77              |
| 5:P16:16:PHE:HE1    | 6:O16:311:LEU:CD1   | 1.93                     | 0.77              |
| 10:C16:1250:ALA:CB  | 10:C16:1309:ARG:NH1 | 2.48                     | 0.77              |
| 11:A24:207:TYR:HB3  | 11:A24:536:HIS:CD2  | 2.20                     | 0.77              |
| 11:A40:1:MET:SD     | 22:I16:151:GLU:OE1  | 2.43                     | 0.77              |
| 11:A40:607:ARG:CZ   | 24:D32:914:PHE:CE1  | 2.68                     | 0.77              |
| 12:A:603:ALA:HB1    | 12:A:616:ARG:HD2    | 1.67                     | 0.77              |
| 14:W:261:TRP:CZ2    | 14:W:265:MET:HE3    | 2.20                     | 0.77              |
| 10:C:1358:ASP:HB3   | 10:C:1361:LYS:HB2   | 1.67                     | 0.77              |
| 18:B:1940:ALA:HB3   | 18:B:1950:ILE:CD1   | 2.14                     | 0.77              |
| 22:I8:207:PRO:C     | 22:I8:209:TRP:H     | 1.93                     | 0.77              |
| 21:H16:322:LEU:HD13 | 23:J16:689:LEU:CG   | 2.14                     | 0.77              |
| 10:C32:1530:PHE:CD1 | 12:A48:132:MET:HE2  | 2.20                     | 0.77              |
| 2:M8:246:ALA:HB3    | 2:M8:247:PRO:HD3    | 1.67                     | 0.77              |
| 5:P8:144:THR:O      | 5:P8:146:SER:N      | 2.17                     | 0.77              |
| 7:Q8:125:TYR:CD1    | 7:Q8:167:GLY:HA2    | 2.19                     | 0.77              |
| 7:Q8:244:ILE:HG23   | 7:Q8:289:TYR:OH     | 1.85                     | 0.77              |
| 5:P16:73:ASN:HB2    | 6:O16:5:MET:SD      | 2.24                     | 0.77              |
| 9:K:614:PHE:C       | 9:K:683:GLN:HE22    | 1.91                     | 0.77              |
| 10:C16:962:PHE:HZ   | 10:C16:997:ILE:HD12 | 1.50                     | 0.77              |
| 10:C24:453:LEU:HB2  | 10:C24:486:LEU:HD23 | 1.67                     | 0.77              |
| 10:C8:960:PHE:CE2   | 10:C8:1138:GLU:CD   | 2.60                     | 0.77              |
| 18:B:690:TRP:CZ3    | 18:B:739:VAL:HG21   | 2.19                     | 0.77              |
| 19:48:109:GLN:O     | 19:48:418:LYS:CE    | 2.32                     | 0.77              |
| 19:48:252:ARG:HG3   | 19:48:281:TRP:CZ2   | 2.19                     | 0.77              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 21:H:361:ARG:NH1    | 22:I:357:GLU:OE2     | 2.18                     | 0.77              |
| 21:H8:366:MET:HE1   | 22:I8:332:MET:HE3    | 1.62                     | 0.77              |
| 10:C32:1272:GLN:CD  | 10:C32:1289:LYS:HD2  | 2.08                     | 0.77              |
| 10:C32:1358:ASP:HB3 | 10:C32:1361:LYS:HB2  | 1.67                     | 0.77              |
| 10:C32:1385:LEU:HB3 | 10:C32:1426:ARG:HH12 | 1.50                     | 0.77              |
| 3:N8:158:TRP:CD2    | 3:N8:179:LEU:CD2     | 2.67                     | 0.77              |
| 2:M16:225:ASP:HB3   | 2:M16:606:GLN:NE2    | 1.99                     | 0.77              |
| 5:P:73:ASN:HB2      | 6:O:5:MET:SD         | 2.24                     | 0.77              |
| 5:P16:158:VAL:CG1   | 5:P16:248:ILE:HG23   | 2.13                     | 0.77              |
| 5:P16:217:PHE:CE1   | 5:P16:221:LEU:HD12   | 2.20                     | 0.77              |
| 7:Q16:183:ARG:NH1   | 7:Q16:231:HIS:HE1    | 1.83                     | 0.77              |
| 9:K8:1048:GLN:CD    | 9:K8:1128:ARG:HG2    | 2.09                     | 0.77              |
| 10:C16:390:HIS:CD2  | 10:C16:452:LEU:HD22  | 2.20                     | 0.77              |
| 10:C16:667:ILE:HG12 | 10:C16:670:GLU:H     | 1.50                     | 0.77              |
| 11:A24:207:TYR:HB3  | 11:A24:536:HIS:NE2   | 2.00                     | 0.77              |
| 10:C24:847:ARG:CZ   | 10:C24:903:ASN:CB    | 2.63                     | 0.77              |
| 10:C24:1548:ILE:CG1 | 24:D24:1407:PHE:CE2  | 2.59                     | 0.77              |
| 11:A40:437:LEU:HD11 | 11:A40:454:LYS:NZ    | 2.00                     | 0.77              |
| 12:A:127:SER:CB     | 10:C:1466:ARG:NH1    | 2.48                     | 0.77              |
| 10:C:627:VAL:CG1    | 10:C:628:GLY:H       | 1.95                     | 0.77              |
| 10:C8:615:GLU:O     | 10:C8:619:LEU:HD12   | 1.85                     | 0.77              |
| 10:C8:1618:SER:O    | 10:C8:1620:ILE:N     | 2.15                     | 0.77              |
| 11:A16:207:TYR:HB3  | 11:A16:536:HIS:CD2   | 2.20                     | 0.77              |
| 11:A16:798:PHE:HE1  | 11:A16:847:ARG:CZ    | 1.91                     | 0.77              |
| 11:A32:603:ALA:HB1  | 11:A32:616:ARG:HD2   | 1.67                     | 0.77              |
| 18:B:132:LEU:HD13   | 18:B:199:LEU:HD11    | 1.67                     | 0.77              |
| 18:B:842:ASN:O      | 18:B:899:LYS:NZ      | 2.17                     | 0.77              |
| 18:B8:132:LEU:HD13  | 18:B8:199:LEU:HD11   | 1.67                     | 0.77              |
| 20:E8:434:TRP:CE2   | 24:D40:72:GLU:CB     | 2.52                     | 0.77              |
| 23:J32:718:GLN:CD   | 23:J32:737:TRP:HZ3   | 1.83                     | 0.77              |
| 21:H8:361:ARG:NH1   | 22:I8:357:GLU:OE2    | 2.18                     | 0.77              |
| 12:A48:207:TYR:HB3  | 12:A48:536:HIS:NE2   | 2.00                     | 0.77              |
| 2:M:254:LEU:HD22    | 2:M:283:ILE:HD11     | 1.67                     | 0.77              |
| 2:M:571:TYR:CD1     | 2:M:595:LEU:HD12     | 2.19                     | 0.77              |
| 2:M:639:GLN:NE2     | 3:N:269:LEU:CD1      | 2.39                     | 0.77              |
| 1:R8:1139:ARG:NH1   | 1:R8:1157:ARG:CZ     | 2.28                     | 0.77              |
| 2:M16:639:GLN:NE2   | 3:N16:269:LEU:CD1    | 2.39                     | 0.77              |
| 5:P:144:THR:O       | 5:P:146:SER:N        | 2.17                     | 0.77              |
| 7:Q8:279:LEU:HD21   | 7:Q8:315:GLY:HA3     | 1.66                     | 0.77              |
| 6:O16:119:ARG:HE    | 6:O16:181:GLU:C      | 1.93                     | 0.77              |
| 8:L16:1069:LEU:CG   | 9:K16:1086:VAL:HG11  | 2.14                     | 0.77              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:K8:894:LYS:HD2    | 9:K8:1058:GLU:CG    | 2.14                     | 0.77              |
| 10:C16:878:ARG:HH21 | 10:C16:885:VAL:HG23 | 1.49                     | 0.77              |
| 10:C16:1466:ARG:NH1 | 11:A24:127:SER:CB   | 2.48                     | 0.77              |
| 10:C16:1541:PHE:HE1 | 10:C16:1649:LYS:HD2 | 1.50                     | 0.77              |
| 10:C24:667:ILE:HG12 | 10:C24:670:GLU:H    | 1.50                     | 0.77              |
| 10:C24:1466:ARG:NH2 | 11:A40:124:ASN:HA   | 2.00                     | 0.77              |
| 11:A40:468:VAL:O    | 11:A40:470:LEU:N    | 2.18                     | 0.77              |
| 14:W:649:LEU:HD11   | 15:J:572:ASP:OD1    | 1.84                     | 0.77              |
| 10:C:453:LEU:HD22   | 10:C:459:LEU:HD22   | 1.60                     | 0.77              |
| 10:C8:764:ILE:HD12  | 10:C8:781:VAL:HG21  | 1.66                     | 0.77              |
| 11:A16:91:GLU:N     | 18:B:1800:ARG:NH2   | 2.32                     | 0.77              |
| 18:B:235:ARG:HH12   | 18:B:308:GLU:CD     | 1.92                     | 0.77              |
| 18:B:313:ILE:CD1    | 18:B:331:TRP:CG     | 2.67                     | 0.77              |
| 18:B:1045:LYS:NZ    | 18:B:1100:LEU:HD23  | 2.00                     | 0.77              |
| 21:H:322:LEU:HD13   | 23:J32:689:LEU:CG   | 2.14                     | 0.77              |
| 21:H:338:MET:HE3    | 23:J32:692:VAL:HG21 | 1.67                     | 0.77              |
| 22:I:171:MET:HE1    | 23:J32:592:VAL:HG13 | 1.67                     | 0.77              |
| 22:I24:171:MET:HE2  | 23:J24:592:VAL:HG13 | 1.65                     | 0.77              |
| 22:I16:131:ARG:HG3  | 23:J16:557:ARG:HH22 | 1.46                     | 0.77              |
| 10:C32:878:ARG:HH21 | 10:C32:885:VAL:HG23 | 1.49                     | 0.77              |
| 12:A48:437:LEU:HD11 | 12:A48:454:LYS:NZ   | 2.00                     | 0.77              |
| 2:M:202:LYS:HZ1     | 2:M:207:SER:C       | 1.93                     | 0.76              |
| 1:R8:1168:LEU:HD23  | 1:R8:1216:ILE:HG13  | 1.66                     | 0.76              |
| 2:M8:202:LYS:HE3    | 2:M8:206:SER:OG     | 1.81                     | 0.76              |
| 2:M16:571:TYR:CD1   | 2:M16:595:LEU:HD12  | 2.19                     | 0.76              |
| 2:M16:627:TYR:CE1   | 3:N16:162:THR:HB    | 2.19                     | 0.76              |
| 5:P:217:PHE:CE1     | 5:P:221:LEU:HD12    | 2.20                     | 0.76              |
| 5:P16:11:GLY:N      | 5:P16:26:TYR:OH     | 2.17                     | 0.76              |
| 9:K8:788:LEU:HD23   | 9:K8:856:ILE:HD11   | 1.64                     | 0.76              |
| 10:C16:847:ARG:CZ   | 10:C16:903:ASN:CB   | 2.63                     | 0.76              |
| 11:A40:54:ASN:HB3   | 11:A40:59:GLN:NE2   | 1.98                     | 0.76              |
| 12:A:246:SER:OG     | 12:A:500:ASP:OD2    | 2.02                     | 0.76              |
| 12:A:437:LEU:HD11   | 12:A:454:LYS:NZ     | 2.00                     | 0.76              |
| 10:C:1283:LEU:HD23  | 10:C:1287:MET:HG3   | 1.65                     | 0.76              |
| 11:A16:603:ALA:HB1  | 11:A16:616:ARG:HD2  | 1.67                     | 0.76              |
| 18:B:13:TRP:HB3     | 18:B:46:TRP:CZ2     | 2.20                     | 0.76              |
| 18:B:603:PHE:HB3    | 18:B:619:ARG:HH12   | 1.50                     | 0.76              |
| 18:B:1069:VAL:HA    | 18:B:1072:LEU:HD12  | 1.66                     | 0.76              |
| 19:4:97:LEU:HD11    | 19:4:232:TYR:CD2    | 2.20                     | 0.76              |
| 19:48:250:ILE:HG12  | 20:E8:165:ARG:NH2   | 2.00                     | 0.76              |
| 20:E8:432:ILE:CG2   | 24:D40:72:GLU:HG2   | 2.15                     | 0.76              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I:207:PRO:C       | 22:I:209:TRP:H       | 1.93                     | 0.76              |
| 21:H8:301:ARG:NH2    | 22:I8:284:GLU:OE2    | 2.18                     | 0.76              |
| 21:H16:361:ARG:NH1   | 22:I16:357:GLU:OE2   | 2.18                     | 0.76              |
| 24:D24:1330:ARG:NH2  | 24:D32:719:ARG:NH1   | 2.32                     | 0.76              |
| 10:C32:1034:SER:N    | 10:C32:1218:ARG:HH22 | 1.81                     | 0.76              |
| 10:C32:1068:THR:O    | 10:C32:1069:TYR:C    | 2.25                     | 0.76              |
| 12:A48:207:TYR:HB3   | 12:A48:536:HIS:CD2   | 2.20                     | 0.76              |
| 2:M8:217:ILE:HD11    | 3:N8:28:THR:HG21     | 1.66                     | 0.76              |
| 2:M8:399:THR:HB      | 2:M8:480:ARG:HH21    | 1.47                     | 0.76              |
| 4:T16:671:ILE:HD13   | 5:P16:699:SER:N      | 2.00                     | 0.76              |
| 5:P:229:ASP:HA       | 5:P:333:GLN:OE1      | 1.85                     | 0.76              |
| 5:P:291:LEU:HD12     | 5:P:299:CYS:SG       | 2.24                     | 0.76              |
| 7:Q8:98:MET:HE2      | 7:Q8:110:VAL:HG11    | 1.67                     | 0.76              |
| 5:P16:16:PHE:HE2     | 5:P16:461:HIS:HE1    | 1.33                     | 0.76              |
| 9:K:792:LEU:HD12     | 9:K:864:ILE:HD13     | 1.23                     | 0.76              |
| 11:A24:212:LYS:HE3   | 11:A24:585:MET:SD    | 2.24                     | 0.76              |
| 10:C24:1074:LEU:CD2  | 18:B8:256:VAL:C      | 2.58                     | 0.76              |
| 10:C24:1358:ASP:HB3  | 10:C24:1361:LYS:HB2  | 1.67                     | 0.76              |
| 10:C24:1549:VAL:HG13 | 10:C24:1592:VAL:CG1  | 2.15                     | 0.76              |
| 11:A40:11:THR:HG21   | 22:I16:162:GLN:HE21  | 1.47                     | 0.76              |
| 12:A:132:MET:HE2     | 10:C:1530:PHE:CD1    | 2.20                     | 0.76              |
| 12:A:212:LYS:HE3     | 12:A:585:MET:SD      | 2.24                     | 0.76              |
| 12:A:557:LEU:HD22    | 12:A:561:ASP:HB3     | 1.67                     | 0.76              |
| 10:C:1424:GLN:NE2    | 10:C:1478:VAL:HG11   | 1.99                     | 0.76              |
| 10:C8:345:MET:HE3    | 10:C8:401:ILE:HD13   | 1.49                     | 0.76              |
| 10:C8:1250:ALA:CB    | 10:C8:1309:ARG:NH1   | 2.48                     | 0.76              |
| 10:C8:1328:PHE:CZ    | 10:C8:1377:ILE:HD11  | 2.18                     | 0.76              |
| 10:C8:1424:GLN:NE2   | 10:C8:1478:VAL:HG11  | 1.99                     | 0.76              |
| 10:C8:1682:VAL:HG21  | 10:C8:1758:LEU:CD2   | 2.16                     | 0.76              |
| 11:A16:437:LEU:HD11  | 11:A16:454:LYS:NZ    | 2.00                     | 0.76              |
| 11:A32:437:LEU:HD11  | 11:A32:454:LYS:NZ    | 2.00                     | 0.76              |
| 11:A32:629:LEU:C     | 11:A32:678:LYS:HZ3   | 1.92                     | 0.76              |
| 11:A32:764:LYS:HE2   | 19:48:36:LYS:HZ2     | 1.49                     | 0.76              |
| 18:B:460:PRO:HB2     | 18:B:562:ARG:HH11    | 1.50                     | 0.76              |
| 18:B:484:TYR:CE2     | 18:B:556:ILE:CD1     | 2.68                     | 0.76              |
| 18:B8:313:ILE:CD1    | 18:B8:331:TRP:CG     | 2.67                     | 0.76              |
| 19:48:100:ILE:CD1    | 19:48:274:PHE:HE1    | 1.97                     | 0.76              |
| 21:H8:321:SER:HB3    | 21:H8:323:TYR:CE1    | 2.19                     | 0.76              |
| 22:I24:171:MET:HE1   | 23:J24:592:VAL:HG13  | 1.68                     | 0.76              |
| 22:I16:300:LEU:CD1   | 23:J16:689:LEU:HD21  | 2.16                     | 0.76              |
| 10:C32:1250:ALA:CB   | 10:C32:1309:ARG:NH1  | 2.48                     | 0.76              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 12:A48:212:LYS:HE3   | 12:A48:585:MET:SD   | 2.24                     | 0.76              |
| 1:R:1381:GLU:O       | 1:R:1382:LYS:CG     | 2.27                     | 0.76              |
| 1:R8:1265:PHE:CD2    | 5:P8:684:ARG:NH1    | 2.53                     | 0.76              |
| 9:K8:950:LYS:HE3     | 9:K8:977:GLU:HB3    | 1.68                     | 0.76              |
| 10:C16:1530:PHE:CD1  | 11:A24:132:MET:HE2  | 2.20                     | 0.76              |
| 11:A24:468:VAL:O     | 11:A24:470:LEU:N    | 2.18                     | 0.76              |
| 10:C24:615:GLU:O     | 10:C24:619:LEU:HD12 | 1.85                     | 0.76              |
| 12:A:207:TYR:HB3     | 12:A:536:HIS:CD2    | 2.20                     | 0.76              |
| 10:C:798:VAL:HG11    | 10:C:802:TRP:CH2    | 2.20                     | 0.76              |
| 10:C:1328:PHE:CZ     | 10:C:1377:ILE:HD11  | 2.18                     | 0.76              |
| 11:A16:90:PHE:HB2    | 18:B:1788:ILE:HD12  | 1.64                     | 0.76              |
| 18:B8:235:ARG:HH12   | 18:B8:308:GLU:CD    | 1.92                     | 0.76              |
| 18:B8:499:ILE:HD11   | 18:B8:545:VAL:HG21  | 1.66                     | 0.76              |
| 22:I8:171:MET:HE1    | 23:J8:592:VAL:HG13  | 1.67                     | 0.76              |
| 22:I8:290:ASP:OD1    | 22:I8:293:LYS:HD2   | 1.85                     | 0.76              |
| 21:H24:322:LEU:HD13  | 23:J24:689:LEU:CG   | 2.14                     | 0.76              |
| 21:H24:361:ARG:NH1   | 22:I24:357:GLU:OE2  | 2.18                     | 0.76              |
| 22:I24:300:LEU:CD1   | 23:J24:689:LEU:HD21 | 2.16                     | 0.76              |
| 24:D16:1099:ARG:HG3  | 24:D16:1101:HIS:NE2 | 2.00                     | 0.76              |
| 10:C32:847:ARG:CZ    | 10:C32:903:ASN:CB   | 2.63                     | 0.76              |
| 1:R:1422:SER:HB2     | 6:O:154:GLN:NE2     | 2.01                     | 0.76              |
| 2:M:225:ASP:HB3      | 2:M:606:GLN:NE2     | 1.99                     | 0.76              |
| 2:M8:669:ALA:HB1     | 2:M8:684:GLN:HG2    | 1.65                     | 0.76              |
| 5:P8:12:GLU:O        | 5:P8:14:VAL:N       | 2.19                     | 0.76              |
| 5:P8:229:ASP:HA      | 5:P8:333:GLN:OE1    | 1.85                     | 0.76              |
| 5:P8:682:ARG:NH2     | 5:P8:689:GLU:OE1    | 2.19                     | 0.76              |
| 5:P16:144:THR:O      | 5:P16:146:SER:N     | 2.17                     | 0.76              |
| 8:L8:1058:ILE:HG23   | 9:K8:1083:ILE:HD11  | 1.67                     | 0.76              |
| 8:L16:173:ASP:HB3    | 12:A48:783:PHE:HE1  | 1.38                     | 0.76              |
| 9:K:975:MET:CE       | 9:K:1005:LEU:HD21   | 2.15                     | 0.76              |
| 10:C16:453:LEU:HB2   | 10:C16:486:LEU:HD23 | 1.67                     | 0.76              |
| 10:C16:1358:ASP:HB3  | 10:C16:1361:LYS:HB2 | 1.67                     | 0.76              |
| 10:C24:1074:LEU:HD21 | 18:B8:256:VAL:CA    | 2.15                     | 0.76              |
| 10:C24:1466:ARG:NH1  | 11:A40:127:SER:CB   | 2.49                     | 0.76              |
| 10:C:615:GLU:O       | 10:C:619:LEU:HD12   | 1.85                     | 0.76              |
| 11:A16:212:LYS:HE3   | 11:A16:585:MET:SD   | 2.24                     | 0.76              |
| 11:A16:665:GLU:HG2   | 24:D16:1462:PHE:CE1 | 2.20                     | 0.76              |
| 11:A32:207:TYR:HB3   | 11:A32:536:HIS:NE2  | 2.00                     | 0.76              |
| 18:B:771:MET:CE      | 18:B:840:VAL:HG11   | 2.13                     | 0.76              |
| 18:B8:603:PHE:HB3    | 18:B8:619:ARG:HH12  | 1.50                     | 0.76              |
| 18:B8:1215:PHE:CZ    | 18:B8:1234:MET:SD   | 2.79                     | 0.76              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1900:ILE:HD11  | 18:B8:1946:LEU:HD22  | 1.66                     | 0.76              |
| 19:4:189:LEU:HD13    | 19:4:203:LEU:HG      | 1.66                     | 0.76              |
| 20:E:353:ILE:CB      | 20:E:413:PHE:CE2     | 2.67                     | 0.76              |
| 20:E:429:PRO:CG      | 24:D:69:VAL:HG22     | 2.15                     | 0.76              |
| 19:48:250:ILE:CD1    | 20:E8:165:ARG:HH21   | 1.93                     | 0.76              |
| 20:E8:447:ILE:CG2    | 20:E8:451:ILE:HG22   | 2.15                     | 0.76              |
| 22:I8:300:LEU:HD22   | 23:J8:689:LEU:HD21   | 1.67                     | 0.76              |
| 21:H24:288:THR:CB    | 23:J24:650:GLN:HE21  | 1.98                     | 0.76              |
| 22:I24:207:PRO:C     | 22:I24:209:TRP:H     | 1.93                     | 0.76              |
| 10:C32:798:VAL:HG11  | 10:C32:802:TRP:CH2   | 2.20                     | 0.76              |
| 12:A48:246:SER:OG    | 12:A48:500:ASP:OD2   | 2.02                     | 0.76              |
| 9:K8:788:LEU:O       | 9:K8:792:LEU:HD13    | 1.85                     | 0.76              |
| 9:K16:894:LYS:HZ1    | 9:K16:1057:GLU:CB    | 1.93                     | 0.76              |
| 10:C16:615:GLU:O     | 10:C16:619:LEU:HD12  | 1.85                     | 0.76              |
| 10:C16:1549:VAL:HG13 | 10:C16:1592:VAL:CG1  | 2.14                     | 0.76              |
| 11:A24:437:LEU:HD11  | 11:A24:454:LYS:NZ    | 2.00                     | 0.76              |
| 10:C24:1385:LEU:HB3  | 10:C24:1426:ARG:HH12 | 1.50                     | 0.76              |
| 11:A40:198:PRO:CB    | 11:A40:200:HIS:CE1   | 2.69                     | 0.76              |
| 10:C:1282:CYS:HA     | 10:C:1738:MET:HE1    | 1.67                     | 0.76              |
| 10:C8:1541:PHE:HE1   | 10:C8:1649:LYS:HD2   | 1.50                     | 0.76              |
| 18:B:603:PHE:CB      | 18:B:619:ARG:NH2     | 2.48                     | 0.76              |
| 18:B:1215:PHE:CZ     | 18:B:1234:MET:SD     | 2.78                     | 0.76              |
| 20:E:447:ILE:CG2     | 20:E:451:ILE:HG22    | 2.15                     | 0.76              |
| 22:I:304:LEU:HB3     | 22:I:305:PRO:HD3     | 1.67                     | 0.76              |
| 21:H8:243:LEU:HD11   | 23:J8:603:LEU:HG     | 1.66                     | 0.76              |
| 21:H8:312:GLN:CG     | 21:H8:316:ILE:CD1    | 2.39                     | 0.76              |
| 22:I16:207:PRO:C     | 22:I16:209:TRP:H     | 1.93                     | 0.76              |
| 22:I16:300:LEU:HD22  | 23:J16:689:LEU:HD21  | 1.67                     | 0.76              |
| 10:C32:345:MET:HE1   | 10:C32:401:ILE:HD13  | 1.41                     | 0.76              |
| 10:C32:1682:VAL:HG21 | 10:C32:1758:LEU:CD2  | 2.16                     | 0.76              |
| 12:A48:198:PRO:CB    | 12:A48:200:HIS:CE1   | 2.69                     | 0.76              |
| 1:R:1188:TYR:CZ      | 24:D:1459:LEU:HB3    | 2.20                     | 0.76              |
| 2:M16:672:TYR:CG     | 2:M16:680:LYS:HD3    | 2.11                     | 0.76              |
| 5:P:394:ASN:C        | 5:P:396:SER:N        | 2.44                     | 0.76              |
| 7:Q:27:GLN:HE22      | 7:Q:33:ARG:HG2       | 1.45                     | 0.76              |
| 7:Q:183:ARG:NH1      | 7:Q:231:HIS:HE1      | 1.83                     | 0.76              |
| 5:P8:217:PHE:CE1     | 5:P8:221:LEU:HD12    | 2.20                     | 0.76              |
| 5:P16:229:ASP:HA     | 5:P16:333:GLN:OE1    | 1.85                     | 0.76              |
| 8:L8:270:LEU:HD21    | 12:A48:155:SER:HB3   | 1.65                     | 0.76              |
| 8:L16:856:LEU:CD2    | 9:K16:1281:SER:OG    | 2.33                     | 0.76              |
| 9:K8:994:TYR:CD2     | 9:K8:1023:LEU:HD11   | 2.21                     | 0.76              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K8:1142:ARG:HH21   | 9:K8:1204:THR:CA     | 1.98                     | 0.76              |
| 11:A24:374:PHE:CE2   | 11:A24:426:ILE:HD12  | 2.21                     | 0.76              |
| 10:C24:1250:ALA:HB2  | 10:C24:1309:ARG:HH12 | 1.48                     | 0.76              |
| 10:C24:1278:ASP:OD2  | 21:H24:283:LYS:HG2   | 1.86                     | 0.76              |
| 11:A40:557:LEU:HD22  | 11:A40:561:ASP:HB3   | 1.67                     | 0.76              |
| 12:A:468:VAL:O       | 12:A:470:LEU:N       | 2.18                     | 0.76              |
| 10:C:1220:SER:HA     | 10:C:1225:ARG:CZ     | 2.16                     | 0.76              |
| 10:C:1624:LEU:CD2    | 10:C:1628:SER:HB2    | 2.16                     | 0.76              |
| 10:C8:1333:HIS:HE1   | 10:C8:1337:LEU:HD23  | 1.51                     | 0.76              |
| 11:A16:1:MET:SD      | 22:I:151:GLU:OE1     | 2.43                     | 0.76              |
| 11:A16:557:LEU:HD22  | 11:A16:561:ASP:HB3   | 1.67                     | 0.76              |
| 11:A32:90:PHE:HB2    | 18:B8:1788:ILE:HD12  | 1.61                     | 0.76              |
| 18:B8:460:PRO:HB2    | 18:B8:562:ARG:HH11   | 1.50                     | 0.76              |
| 18:B8:1045:LYS:NZ    | 18:B8:1100:LEU:HD23  | 2.00                     | 0.76              |
| 18:B8:1069:VAL:HA    | 18:B8:1072:LEU:HD12  | 1.66                     | 0.76              |
| 19:48:189:LEU:HD13   | 19:48:203:LEU:HG     | 1.66                     | 0.76              |
| 21:H24:338:MET:HE3   | 23:J24:692:VAL:HG21  | 1.67                     | 0.76              |
| 2:M8:639:GLN:NE2     | 3:N8:269:LEU:CD1     | 2.39                     | 0.76              |
| 5:P16:467:GLN:NE2    | 6:O16:291:SER:CB     | 2.49                     | 0.76              |
| 10:C16:1282:CYS:HA   | 10:C16:1738:MET:HE1  | 1.68                     | 0.76              |
| 10:C16:1615:PHE:HB2  | 10:C16:1674:LEU:CD2  | 2.16                     | 0.76              |
| 11:A24:323:LEU:HD21  | 17:F:74:ILE:HD12     | 1.68                     | 0.76              |
| 10:C24:1530:PHE:CD1  | 11:A40:132:MET:HE2   | 2.20                     | 0.76              |
| 10:C24:1624:LEU:HD23 | 10:C24:1628:SER:HB2  | 1.64                     | 0.76              |
| 10:C24:1691:GLU:OE1  | 23:J24:735:LYS:HA    | 1.85                     | 0.76              |
| 10:C24:1814:LYS:NZ   | 23:J24:738:MET:HB2   | 2.00                     | 0.76              |
| 14:W:715:ASP:OD1     | 10:C8:1568:ARG:NE    | 2.19                     | 0.76              |
| 10:C:1682:VAL:HG21   | 10:C:1758:LEU:CD2    | 2.16                     | 0.76              |
| 10:C8:664:ASN:HA     | 10:C8:667:ILE:CG1    | 2.16                     | 0.76              |
| 10:C8:761:VAL:HG21   | 10:C8:826:TYR:HA     | 1.65                     | 0.76              |
| 10:C8:878:ARG:HH21   | 10:C8:885:VAL:HG23   | 1.49                     | 0.76              |
| 10:C8:1385:LEU:HB3   | 10:C8:1426:ARG:HH12  | 1.50                     | 0.76              |
| 10:C8:1615:PHE:HB2   | 10:C8:1674:LEU:CD2   | 2.16                     | 0.76              |
| 10:C8:1624:LEU:CD2   | 10:C8:1628:SER:HB2   | 2.16                     | 0.76              |
| 11:A16:98:ALA:O      | 18:B:1103:LYS:NZ     | 2.18                     | 0.76              |
| 11:A16:207:TYR:HB3   | 11:A16:536:HIS:NE2   | 2.00                     | 0.76              |
| 18:B8:1342:LEU:CD2   | 18:B8:1406:ALA:HB1   | 2.14                     | 0.76              |
| 18:B8:1618:HIS:CE1   | 18:B8:1622:ILE:CD1   | 2.61                     | 0.76              |
| 10:C32:1466:ARG:NH1  | 12:A48:127:SER:CB    | 2.48                     | 0.76              |
| 12:A48:437:LEU:HD11  | 12:A48:454:LYS:HZ3   | 1.51                     | 0.76              |
| 2:M:844:VAL:HG23     | 4:T:660:LEU:HD21     | 1.59                     | 0.76              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M16:202:LYS:HZ1   | 2:M16:207:SER:C     | 1.93                     | 0.76              |
| 7:Q8:98:MET:CE      | 7:Q8:110:VAL:HG11   | 2.16                     | 0.76              |
| 9:K:994:TYR:CD2     | 9:K:1023:LEU:HD11   | 2.21                     | 0.76              |
| 9:K8:955:TYR:HE1    | 9:K8:985:PHE:HB2    | 1.48                     | 0.76              |
| 10:C16:764:ILE:HD12 | 10:C16:781:VAL:HG21 | 1.66                     | 0.76              |
| 10:C16:798:VAL:HG11 | 10:C16:802:TRP:CH2  | 2.20                     | 0.76              |
| 11:A24:11:THR:HG21  | 22:I8:162:GLN:HE21  | 1.47                     | 0.76              |
| 10:C24:1250:ALA:CB  | 10:C24:1309:ARG:NH1 | 2.48                     | 0.76              |
| 10:C24:1615:PHE:HB2 | 10:C24:1674:LEU:CD2 | 2.16                     | 0.76              |
| 11:A40:749:GLN:NE2  | 24:D24:1398:ARG:NE  | 2.34                     | 0.76              |
| 13:V:818:THR:HA     | 13:V:824:TRP:NE1    | 1.99                     | 0.76              |
| 14:W:584:CYS:SG     | 15:J:573:LYS:HD2    | 2.25                     | 0.76              |
| 10:C:345:MET:HE3    | 10:C:401:ILE:HD13   | 1.50                     | 0.76              |
| 10:C:453:LEU:HB2    | 10:C:486:LEU:HD23   | 1.67                     | 0.76              |
| 10:C8:1282:CYS:HA   | 10:C8:1738:MET:HE1  | 1.67                     | 0.76              |
| 11:A32:98:ALA:O     | 18:B8:1103:LYS:NZ   | 2.18                     | 0.76              |
| 11:A32:468:VAL:O    | 11:A32:470:LEU:N    | 2.18                     | 0.76              |
| 18:B:671:MET:HE2    | 18:B:736:ALA:HB2    | 1.67                     | 0.76              |
| 18:B:1649:SER:O     | 18:B:1653:LEU:HB2   | 1.85                     | 0.76              |
| 18:B8:484:TYR:CE2   | 18:B8:556:ILE:CD1   | 2.68                     | 0.76              |
| 19:4:365:GLU:CD     | 19:4:442:ARG:HH21   | 1.92                     | 0.76              |
| 20:E:49:THR:HA      | 20:E:121:VAL:HG11   | 1.68                     | 0.76              |
| 21:H:262:GLU:OE1    | 23:J32:648:TYR:OH   | 2.04                     | 0.76              |
| 22:I8:199:PHE:HB3   | 23:J8:620:MET:SD    | 2.24                     | 0.76              |
| 22:I24:304:LEU:HB3  | 22:I24:305:PRO:HD3  | 1.68                     | 0.76              |
| 10:C32:615:GLU:O    | 10:C32:619:LEU:HD12 | 1.85                     | 0.76              |
| 10:C32:764:ILE:HD12 | 10:C32:781:VAL:HG21 | 1.66                     | 0.76              |
| 2:M8:730:GLU:CD     | 8:L16:504:GLN:NE2   | 2.44                     | 0.76              |
| 2:M16:672:TYR:CD2   | 2:M16:680:LYS:CE    | 2.68                     | 0.76              |
| 5:P:607:PHE:CZ      | 5:P:633:LEU:HD13    | 2.21                     | 0.76              |
| 9:K8:853:ALA:HB1    | 9:K8:856:ILE:HD12   | 1.68                     | 0.76              |
| 10:C16:1220:SER:HA  | 10:C16:1225:ARG:CZ  | 2.16                     | 0.76              |
| 10:C24:1220:SER:HA  | 10:C24:1225:ARG:CZ  | 2.16                     | 0.76              |
| 10:C24:1333:HIS:HE1 | 10:C24:1337:LEU:CD2 | 1.99                     | 0.76              |
| 11:A40:629:LEU:C    | 11:A40:678:LYS:HZ3  | 1.93                     | 0.76              |
| 12:A:374:PHE:CE2    | 12:A:426:ILE:HD12   | 2.21                     | 0.76              |
| 14:W:698:LEU:HD12   | 15:J:617:LEU:CD2    | 2.15                     | 0.76              |
| 10:C:1050:HIS:CD2   | 10:C:1086:LYS:HZ1   | 1.88                     | 0.76              |
| 10:C:1154:TRP:CZ2   | 10:C:1158:HIS:NE2   | 2.54                     | 0.76              |
| 10:C8:453:LEU:CD2   | 10:C8:459:LEU:HD11  | 2.08                     | 0.76              |
| 10:C8:847:ARG:CZ    | 10:C8:903:ASN:CB    | 2.63                     | 0.76              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:587:VAL:HG21  | 11:A32:636:PHE:HE1   | 1.51                     | 0.76              |
| 18:B:410:GLN:HE21    | 18:B:538:ARG:HH21    | 1.33                     | 0.76              |
| 18:B:428:GLN:CG      | 18:B:584:ARG:CZ      | 2.46                     | 0.76              |
| 18:B:1342:LEU:CD2    | 18:B:1406:ALA:HB1    | 2.13                     | 0.76              |
| 18:B8:410:GLN:HE21   | 18:B8:538:ARG:HH21   | 1.33                     | 0.76              |
| 22:I24:300:LEU:HD22  | 23:J24:689:LEU:HD21  | 1.67                     | 0.76              |
| 21:H16:243:LEU:HD11  | 23:J16:603:LEU:HG    | 1.66                     | 0.76              |
| 10:C32:627:VAL:CG1   | 10:C32:628:GLY:H     | 1.95                     | 0.76              |
| 2:M:202:LYS:HE3      | 2:M:206:SER:OG       | 1.81                     | 0.76              |
| 5:P:16:PHE:HE1       | 6:O:311:LEU:CD1      | 1.93                     | 0.76              |
| 5:P:578:LEU:HD11     | 5:P:608:LYS:HD3      | 1.68                     | 0.76              |
| 6:O8:119:ARG:HE      | 6:O8:181:GLU:C       | 1.93                     | 0.76              |
| 5:P16:578:LEU:HD11   | 5:P16:608:LYS:HD3    | 1.68                     | 0.76              |
| 7:Q16:219:GLY:HA2    | 7:Q16:221:TRP:HE1    | 1.50                     | 0.76              |
| 10:C16:407:LYS:CE    | 10:C16:465:PHE:HE2   | 1.93                     | 0.76              |
| 10:C16:1285:VAL:HG21 | 10:C16:1738:MET:HE3  | 1.61                     | 0.76              |
| 10:C16:1303:LEU:HD13 | 10:C16:1323:LEU:CD2  | 2.16                     | 0.76              |
| 10:C16:1333:HIS:HE1  | 10:C16:1337:LEU:CD2  | 1.99                     | 0.76              |
| 11:A24:198:PRO:CB    | 11:A24:200:HIS:CE1   | 2.69                     | 0.76              |
| 11:A24:603:ALA:HB1   | 11:A24:616:ARG:HD2   | 1.67                     | 0.76              |
| 10:C24:847:ARG:NH2   | 10:C24:911:ILE:H     | 1.84                     | 0.76              |
| 12:A:124:ASN:HA      | 10:C:1466:ARG:NH2    | 2.00                     | 0.76              |
| 10:C:847:ARG:CZ      | 10:C:903:ASN:CB      | 2.63                     | 0.76              |
| 10:C8:1220:SER:HA    | 10:C8:1225:ARG:CZ    | 2.16                     | 0.76              |
| 17:F16:71:GLU:C      | 17:F16:73:GLY:N      | 2.42                     | 0.76              |
| 17:F16:74:ILE:C      | 17:F16:76:ASP:N      | 2.38                     | 0.76              |
| 18:B8:1725:THR:CG2   | 18:B8:1830:LEU:HD22  | 2.15                     | 0.76              |
| 18:B8:1803:THR:C     | 18:B8:1805:GLU:N     | 2.41                     | 0.76              |
| 18:B8:1831:LEU:HD12  | 18:B8:1902:THR:HG23  | 1.66                     | 0.76              |
| 21:H16:288:THR:CB    | 23:J16:650:GLN:HE21  | 1.98                     | 0.76              |
| 10:C32:1045:GLN:O    | 10:C32:1049:SER:OG   | 2.04                     | 0.76              |
| 12:A48:629:LEU:C     | 12:A48:678:LYS:HZ3   | 1.94                     | 0.76              |
| 1:R:1078:SER:HB2     | 5:P:713:LEU:CD2      | 2.12                     | 0.75              |
| 1:R8:1101:ARG:NE     | 24:D40:1459:LEU:O    | 2.19                     | 0.75              |
| 6:O:119:ARG:HE       | 6:O:181:GLU:C        | 1.93                     | 0.75              |
| 5:P8:16:PHE:HE2      | 5:P8:461:HIS:HE1     | 1.34                     | 0.75              |
| 8:L16:173:ASP:OD2    | 12:A48:797:VAL:HG13  | 1.86                     | 0.75              |
| 9:K8:649:MET:CG      | 9:K8:704:ARG:HH22    | 1.99                     | 0.75              |
| 10:C24:225:LEU:HD21  | 10:C24:388:TYR:OH    | 1.87                     | 0.75              |
| 10:C24:1303:LEU:CD1  | 10:C24:1323:LEU:HD23 | 2.17                     | 0.75              |
| 10:C24:1328:PHE:CZ   | 10:C24:1377:ILE:HD11 | 2.18                     | 0.75              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C8:1333:HIS:HE1   | 10:C8:1337:LEU:CD2   | 1.99                     | 0.75              |
| 10:C8:1466:ARG:NH1   | 16:A8:127:SER:CB     | 2.48                     | 0.75              |
| 11:A16:587:VAL:HG21  | 11:A16:636:PHE:HE1   | 1.51                     | 0.75              |
| 11:A32:43:LEU:HD23   | 23:J24:700:LEU:HD23  | 1.67                     | 0.75              |
| 18:B:499:ILE:HD11    | 18:B:545:VAL:HG21    | 1.66                     | 0.75              |
| 18:B8:856:LEU:HD23   | 18:B8:860:HIS:HB3    | 1.68                     | 0.75              |
| 19:48:97:LEU:HD11    | 19:48:232:TYR:CD2    | 2.20                     | 0.75              |
| 19:48:251:ARG:HH21   | 19:48:254:LEU:HD23   | 1.50                     | 0.75              |
| 22:I24:199:PHE:HB3   | 23:J24:620:MET:SD    | 2.24                     | 0.75              |
| 10:C32:453:LEU:HD22  | 10:C32:459:LEU:HD22  | 1.60                     | 0.75              |
| 2:M8:627:TYR:CD2     | 3:N8:167:LEU:CA      | 2.68                     | 0.75              |
| 3:N8:19:MET:CE       | 3:N8:23:GLY:C        | 2.50                     | 0.75              |
| 5:P:188:LEU:CD2      | 5:P:380:MET:HE1      | 2.16                     | 0.75              |
| 7:Q:149:VAL:CG2      | 7:Q:187:TRP:CZ2      | 2.70                     | 0.75              |
| 5:P8:614:VAL:HG23    | 5:P8:629:ARG:HH21    | 1.49                     | 0.75              |
| 7:Q8:149:VAL:CG2     | 7:Q8:187:TRP:CZ2     | 2.70                     | 0.75              |
| 8:L8:1092:LEU:HD13   | 9:K8:999:PHE:CD2     | 2.20                     | 0.75              |
| 9:K:1085:TYR:CZ      | 9:K:1093:SER:HB2     | 2.14                     | 0.75              |
| 9:K8:1214:TYR:OH     | 9:K8:1230:LEU:O      | 2.03                     | 0.75              |
| 10:C16:1133:ILE:HG13 | 10:C16:1152:LYS:HZ2  | 1.50                     | 0.75              |
| 10:C24:1352:GLN:OE1  | 10:C24:1357:LEU:HD12 | 1.87                     | 0.75              |
| 10:C24:1615:PHE:CB   | 10:C24:1674:LEU:HD23 | 2.17                     | 0.75              |
| 11:A40:374:PHE:CE2   | 11:A40:426:ILE:HD12  | 2.21                     | 0.75              |
| 13:V:787:ILE:CD1     | 15:J:592:VAL:CG1     | 2.64                     | 0.75              |
| 10:C:1045:GLN:O      | 10:C:1049:SER:OG     | 2.04                     | 0.75              |
| 10:C8:847:ARG:NH2    | 10:C8:911:ILE:H      | 1.84                     | 0.75              |
| 18:B:609:TYR:CE2     | 18:B:610:VAL:HG22    | 2.21                     | 0.75              |
| 18:B:958:ARG:HG3     | 18:B:1029:THR:CG2    | 2.16                     | 0.75              |
| 21:H:312:GLN:HE22    | 22:I:290:ASP:CB      | 1.99                     | 0.75              |
| 21:H8:262:GLU:OE1    | 23:J8:648:TYR:OH     | 2.04                     | 0.75              |
| 21:H16:262:GLU:OE1   | 23:J16:648:TYR:OH    | 2.04                     | 0.75              |
| 24:D:1:MET:HB2       | 24:D:882:GLU:CD      | 2.11                     | 0.75              |
| 10:C32:1624:LEU:CD2  | 10:C32:1628:SER:HB2  | 2.15                     | 0.75              |
| 1:R:1486:SER:HA      | 2:M:177:VAL:HG23     | 1.69                     | 0.75              |
| 2:M:399:THR:CG2      | 2:M:480:ARG:NH2      | 2.41                     | 0.75              |
| 2:M8:403:LEU:HD21    | 2:M8:425:ALA:HB3     | 1.67                     | 0.75              |
| 2:M16:185:ARG:HH12   | 2:M16:213:LEU:HD12   | 1.51                     | 0.75              |
| 2:M16:833:GLU:HG3    | 2:M16:836:ARG:HH21   | 1.51                     | 0.75              |
| 7:Q:341:GLN:HG2      | 10:C8:751:ARG:HH11   | 1.42                     | 0.75              |
| 7:Q8:219:GLY:HA2     | 7:Q8:221:TRP:HE1     | 1.50                     | 0.75              |
| 7:Q16:98:MET:HE2     | 7:Q16:110:VAL:HG11   | 1.67                     | 0.75              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 8:L8:1092:LEU:CD1    | 9:K8:999:PHE:HD2     | 1.99                     | 0.75              |
| 9:K:1142:ARG:HH21    | 9:K:1204:THR:HA      | 1.48                     | 0.75              |
| 10:C16:8:VAL:HG23    | 10:C16:133:THR:OG1   | 1.86                     | 0.75              |
| 10:C16:1466:ARG:NH2  | 11:A24:124:ASN:HA    | 2.00                     | 0.75              |
| 10:C16:1615:PHE:CB   | 10:C16:1674:LEU:HD23 | 2.17                     | 0.75              |
| 11:A24:107:GLN:NE2   | 21:H8:325:PRO:HA     | 2.02                     | 0.75              |
| 10:C24:798:VAL:HG11  | 10:C24:802:TRP:CH2   | 2.20                     | 0.75              |
| 10:C24:1282:CYS:HA   | 10:C24:1738:MET:HE1  | 1.67                     | 0.75              |
| 10:C24:1682:VAL:HG21 | 10:C24:1758:LEU:CD2  | 2.16                     | 0.75              |
| 11:A40:736:PRO:HB2   | 24:D32:871:ARG:CZ    | 2.16                     | 0.75              |
| 10:C:407:LYS:NZ      | 10:C:465:PHE:CE2     | 2.54                     | 0.75              |
| 10:C:1283:LEU:HD11   | 10:C:1357:LEU:CD1    | 2.17                     | 0.75              |
| 10:C:1352:GLN:OE1    | 10:C:1357:LEU:HD12   | 1.87                     | 0.75              |
| 11:A16:698:LYS:HD3   | 24:D16:1392:MET:O    | 1.86                     | 0.75              |
| 17:F24:71:GLU:C      | 17:F24:73:GLY:N      | 2.42                     | 0.75              |
| 18:B:1264:GLN:NE2    | 18:B:1394:TRP:HZ3    | 1.84                     | 0.75              |
| 18:B8:958:ARG:HG3    | 18:B8:1029:THR:HG21  | 1.68                     | 0.75              |
| 19:48:365:GLU:CD     | 19:48:442:ARG:HH21   | 1.92                     | 0.75              |
| 22:I:300:LEU:HD22    | 23:J32:689:LEU:HD21  | 1.67                     | 0.75              |
| 21:H24:312:GLN:HE22  | 22:I24:290:ASP:CB    | 1.99                     | 0.75              |
| 12:A48:354:ARG:HA    | 12:A48:452:TRP:CZ2   | 2.22                     | 0.75              |
| 1:R:1059:ILE:HG21    | 24:D:1435:ARG:NH2    | 2.01                     | 0.75              |
| 2:M:762:LEU:CG       | 2:M:813:ASN:HD22     | 2.00                     | 0.75              |
| 2:M8:816:ARG:HH12    | 2:M8:849:LEU:CA      | 1.99                     | 0.75              |
| 2:M16:755:THR:C      | 2:M16:757:VAL:H      | 1.95                     | 0.75              |
| 7:Q:98:MET:CE        | 7:Q:110:VAL:HG11     | 2.16                     | 0.75              |
| 5:P8:105:ARG:CD      | 5:P8:130:VAL:HG22    | 2.15                     | 0.75              |
| 5:P8:578:LEU:HD11    | 5:P8:608:LYS:HD3     | 1.68                     | 0.75              |
| 9:K:950:LYS:HE3      | 9:K:977:GLU:HB3      | 1.68                     | 0.75              |
| 9:K:1056:VAL:CG1     | 9:K:1059:ARG:HE      | 1.98                     | 0.75              |
| 10:C16:1283:LEU:HD11 | 10:C16:1357:LEU:CD1  | 2.16                     | 0.75              |
| 10:C16:1290:HIS:CG   | 10:C16:1334:MET:CE   | 2.69                     | 0.75              |
| 11:A24:354:ARG:HA    | 11:A24:452:TRP:CZ2   | 2.22                     | 0.75              |
| 11:A40:43:LEU:HD23   | 23:J16:700:LEU:HD23  | 1.67                     | 0.75              |
| 15:J:722:LEU:HD13    | 10:C8:1623:ILE:HD13  | 1.67                     | 0.75              |
| 11:A16:43:LEU:HD23   | 23:J32:700:LEU:HD23  | 1.67                     | 0.75              |
| 18:B:958:ARG:HG3     | 18:B:1029:THR:HG21   | 1.68                     | 0.75              |
| 18:B8:1291:LEU:CD1   | 18:B8:1332:VAL:CG2   | 2.64                     | 0.75              |
| 18:B8:1649:SER:O     | 18:B8:1653:LEU:HB2   | 1.85                     | 0.75              |
| 20:E:8:GLU:HA        | 20:E:278:GLU:OE1     | 1.87                     | 0.75              |
| 23:J8:718:GLN:CD     | 23:J8:737:TRP:HZ3    | 1.83                     | 0.75              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I24:290:ASP:OD1   | 22:I24:293:LYS:HD2   | 1.85                     | 0.75              |
| 22:I16:171:MET:HE1   | 23:J16:592:VAL:HG13  | 1.67                     | 0.75              |
| 10:C32:1220:SER:HA   | 10:C32:1225:ARG:CZ   | 2.16                     | 0.75              |
| 10:C32:1283:LEU:HD11 | 10:C32:1357:LEU:CD1  | 2.17                     | 0.75              |
| 10:C32:1303:LEU:HD13 | 10:C32:1323:LEU:CD2  | 2.16                     | 0.75              |
| 12:A48:603:ALA:HB1   | 12:A48:616:ARG:HD2   | 1.67                     | 0.75              |
| 1:R:1165:MET:SD      | 5:P:676:GLN:NE2      | 2.60                     | 0.75              |
| 1:R8:1188:TYR:CE2    | 24:D40:1459:LEU:HB3  | 2.22                     | 0.75              |
| 2:M16:593:HIS:HD2    | 3:N16:224:LEU:HD22   | 1.49                     | 0.75              |
| 2:M16:672:TYR:HD2    | 2:M16:680:LYS:HD3    | 1.50                     | 0.75              |
| 3:N16:19:MET:HE2     | 3:N16:23:GLY:HA2     | 1.65                     | 0.75              |
| 7:Q16:279:LEU:HD21   | 7:Q16:315:GLY:HA3    | 1.66                     | 0.75              |
| 9:K8:1085:TYR:HE1    | 9:K8:1093:SER:C      | 1.95                     | 0.75              |
| 10:C16:390:HIS:CD2   | 10:C16:449:GLU:CB    | 2.70                     | 0.75              |
| 10:C16:1624:LEU:CD2  | 10:C16:1628:SER:HB2  | 2.16                     | 0.75              |
| 11:A24:468:VAL:HG21  | 24:D16:1100:GLN:HB3  | 1.67                     | 0.75              |
| 11:A24:504:TYR:HB3   | 11:A24:505:PRO:HD3   | 1.69                     | 0.75              |
| 10:C24:1283:LEU:HD11 | 10:C24:1357:LEU:CD1  | 2.16                     | 0.75              |
| 10:C24:1290:HIS:CG   | 10:C24:1334:MET:CE   | 2.70                     | 0.75              |
| 10:C24:1333:HIS:HE1  | 10:C24:1337:LEU:HD23 | 1.50                     | 0.75              |
| 10:C8:8:VAL:HG23     | 10:C8:133:THR:OG1    | 1.86                     | 0.75              |
| 10:C8:810:ASP:O      | 10:C8:814:SER:OG     | 2.05                     | 0.75              |
| 10:C8:1549:VAL:HG13  | 10:C8:1592:VAL:CG1   | 2.14                     | 0.75              |
| 11:A16:374:PHE:CE2   | 11:A16:426:ILE:HD12  | 2.21                     | 0.75              |
| 11:A16:504:TYR:HB3   | 11:A16:505:PRO:HD3   | 1.69                     | 0.75              |
| 17:F:74:ILE:C        | 17:F:76:ASP:N        | 2.38                     | 0.75              |
| 11:A32:557:LEU:HD22  | 11:A32:561:ASP:HB3   | 1.67                     | 0.75              |
| 18:B8:202:LEU:HD13   | 18:B8:820:ARG:NH1    | 2.02                     | 0.75              |
| 18:B8:1264:GLN:NE2   | 18:B8:1394:TRP:HZ3   | 1.84                     | 0.75              |
| 19:48:188:ALA:C      | 19:48:190:ARG:N      | 2.45                     | 0.75              |
| 22:I:300:LEU:CD1     | 23:J32:689:LEU:HD21  | 2.16                     | 0.75              |
| 21:H8:338:MET:HE3    | 23:J8:692:VAL:HG21   | 1.67                     | 0.75              |
| 21:H24:262:GLU:OE1   | 23:J24:648:TYR:OH    | 2.04                     | 0.75              |
| 21:H16:338:MET:HE3   | 23:J16:692:VAL:HG21  | 1.67                     | 0.75              |
| 12:A48:374:PHE:CE2   | 12:A48:426:ILE:HD12  | 2.21                     | 0.75              |
| 1:R16:1486:SER:HA    | 2:M16:177:VAL:HG23   | 1.69                     | 0.75              |
| 2:M16:627:TYR:CE1    | 3:N16:162:THR:CB     | 2.70                     | 0.75              |
| 2:M16:627:TYR:HD2    | 2:M16:627:TYR:N      | 1.80                     | 0.75              |
| 5:P8:16:PHE:HE1      | 6:O8:311:LEU:CD1     | 1.93                     | 0.75              |
| 7:Q8:183:ARG:NH1     | 7:Q8:231:HIS:HE1     | 1.83                     | 0.75              |
| 9:K:1085:TYR:HE1     | 9:K:1093:SER:C       | 1.95                     | 0.75              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K8:828:PRO:HB2    | 9:K8:830:HIS:CE1     | 2.22                     | 0.75              |
| 10:C24:8:VAL:HG23   | 10:C24:133:THR:OG1   | 1.87                     | 0.75              |
| 10:C24:810:ASP:O    | 10:C24:814:SER:OG    | 2.05                     | 0.75              |
| 12:A:587:VAL:HG21   | 12:A:636:PHE:HE1     | 1.52                     | 0.75              |
| 14:W:586:ILE:HD11   | 15:J:572:ASP:OD2     | 1.86                     | 0.75              |
| 10:C:390:HIS:HB3    | 10:C:452:LEU:HB2     | 1.65                     | 0.75              |
| 10:C8:1283:LEU:HD11 | 10:C8:1357:LEU:CD1   | 2.17                     | 0.75              |
| 10:C8:1352:GLN:OE1  | 10:C8:1357:LEU:HD12  | 1.87                     | 0.75              |
| 18:B:856:LEU:HD23   | 18:B:860:HIS:HB3     | 1.68                     | 0.75              |
| 18:B8:603:PHE:CB    | 18:B8:619:ARG:NH2    | 2.48                     | 0.75              |
| 18:B8:958:ARG:HG3   | 18:B8:1029:THR:CG2   | 2.16                     | 0.75              |
| 22:I:199:PHE:HB3    | 23:J32:620:MET:SD    | 2.24                     | 0.75              |
| 22:I8:300:LEU:CD1   | 23:J8:689:LEU:HD21   | 2.16                     | 0.75              |
| 24:D40:839:GLU:O    | 24:D40:971:HIS:HE1   | 1.68                     | 0.75              |
| 10:C32:1352:GLN:OE1 | 10:C32:1357:LEU:HD12 | 1.86                     | 0.75              |
| 1:R:634:ARG:HD3     | 4:T:160:HIS:CE1      | 2.19                     | 0.75              |
| 2:M8:816:ARG:HH11   | 2:M8:850:TYR:N       | 1.85                     | 0.75              |
| 2:M16:246:ALA:HB3   | 2:M16:247:PRO:HD3    | 1.67                     | 0.75              |
| 2:M16:345:ASP:C     | 2:M16:347:LYS:N      | 2.31                     | 0.75              |
| 4:T16:160:HIS:NE2   | 4:T16:160:HIS:CE1    | 2.55                     | 0.75              |
| 5:P:159:ILE:HD11    | 5:P:214:LEU:HB3      | 1.69                     | 0.75              |
| 5:P16:12:GLU:O      | 5:P16:14:VAL:N       | 2.19                     | 0.75              |
| 5:P16:188:LEU:CD2   | 5:P16:380:MET:HE1    | 2.17                     | 0.75              |
| 9:K:649:MET:CG      | 9:K:704:ARG:HH22     | 1.99                     | 0.75              |
| 10:C16:65:PRO:CG    | 10:C16:96:ARG:NH2    | 2.45                     | 0.75              |
| 10:C16:847:ARG:NH2  | 10:C16:911:ILE:H     | 1.84                     | 0.75              |
| 10:C24:962:PHE:HZ   | 10:C24:997:ILE:HD12  | 1.50                     | 0.75              |
| 10:C24:1541:PHE:HE1 | 10:C24:1649:LYS:HD2  | 1.50                     | 0.75              |
| 12:A:354:ARG:HA     | 12:A:452:TRP:CZ2     | 2.22                     | 0.75              |
| 14:W:517:GLU:CG     | 14:W:605:ASN:O       | 2.21                     | 0.75              |
| 10:C:979:MET:HE1    | 10:C:1028:ILE:CG2    | 2.14                     | 0.75              |
| 10:C:1333:HIS:HE1   | 10:C:1337:LEU:CD2    | 2.00                     | 0.75              |
| 10:C:1385:LEU:HB3   | 10:C:1426:ARG:HH12   | 1.50                     | 0.75              |
| 11:A32:91:GLU:CB    | 18:B8:1112:LYS:HZ1   | 1.86                     | 0.75              |
| 11:A32:374:PHE:CE2  | 11:A32:426:ILE:HD12  | 2.21                     | 0.75              |
| 18:B:202:LEU:HD13   | 18:B:820:ARG:NH1     | 2.02                     | 0.75              |
| 18:B:603:PHE:HB3    | 18:B:619:ARG:NH1     | 2.02                     | 0.75              |
| 24:D:409:LEU:HD13   | 24:D16:746:ALA:HA    | 0.76                     | 0.75              |
| 24:D:1099:ARG:NH2   | 24:D:1149:VAL:CG2    | 2.49                     | 0.75              |
| 10:C32:8:VAL:HG23   | 10:C32:133:THR:OG1   | 1.86                     | 0.75              |
| 10:C32:1303:LEU:CD1 | 10:C32:1323:LEU:HD23 | 2.16                     | 0.75              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1615:PHE:HB2  | 10:C32:1674:LEU:CD2  | 2.16                     | 0.75              |
| 2:M8:351:ALA:HB1     | 8:L8:219:ILE:HG21    | 0.76                     | 0.75              |
| 7:Q:124:PHE:HD1      | 7:Q:125:TYR:CD2      | 2.03                     | 0.75              |
| 8:L16:177:ARG:HG2    | 12:A48:744:GLU:CD    | 2.11                     | 0.75              |
| 8:L16:1030:LEU:HD13  | 9:K16:1285:GLU:CB    | 2.04                     | 0.75              |
| 10:C16:1682:VAL:HG21 | 10:C16:1758:LEU:CD2  | 2.16                     | 0.75              |
| 11:A40:103:GLU:OE1   | 21:H16:323:TYR:CZ    | 2.39                     | 0.75              |
| 11:A40:354:ARG:HA    | 11:A40:452:TRP:CZ2   | 2.22                     | 0.75              |
| 11:A40:504:TYR:HB3   | 11:A40:505:PRO:HD3   | 1.69                     | 0.75              |
| 11:A40:607:ARG:NH2   | 24:D32:914:PHE:HD1   | 1.82                     | 0.75              |
| 12:A:198:PRO:CB      | 12:A:200:HIS:CE1     | 2.69                     | 0.75              |
| 13:V:800:LYS:HB3     | 14:W:688:HIS:NE2     | 2.02                     | 0.75              |
| 14:W:584:CYS:SG      | 15:J:573:LYS:HG3     | 2.27                     | 0.75              |
| 14:W:701:LEU:CD1     | 15:J:624:ALA:CB      | 2.61                     | 0.75              |
| 10:C:8:VAL:HG23      | 10:C:133:THR:OG1     | 1.86                     | 0.75              |
| 10:C:1303:LEU:CD1    | 10:C:1323:LEU:HD23   | 2.16                     | 0.75              |
| 10:C:1333:HIS:HE1    | 10:C:1337:LEU:HD23   | 1.51                     | 0.75              |
| 10:C:1626:GLN:HE21   | 10:C:1692:LYS:HZ3    | 1.33                     | 0.75              |
| 10:C8:1530:PHE:CD1   | 16:A8:132:MET:HE2    | 2.20                     | 0.75              |
| 11:A16:354:ARG:HA    | 11:A16:452:TRP:CZ2   | 2.22                     | 0.75              |
| 17:F8:71:GLU:C       | 17:F8:73:GLY:N       | 2.42                     | 0.75              |
| 11:A32:703:ALA:O     | 24:D32:1398:ARG:NH1  | 2.20                     | 0.75              |
| 18:B:1291:LEU:CD1    | 18:B:1332:VAL:CG2    | 2.64                     | 0.75              |
| 18:B:1831:LEU:HD12   | 18:B:1902:THR:HG23   | 1.66                     | 0.75              |
| 18:B8:536:ILE:HG23   | 18:B8:545:VAL:HG12   | 1.68                     | 0.75              |
| 18:B8:1563:PHE:CZ    | 18:B8:1567:ILE:HD11  | 2.22                     | 0.75              |
| 19:4:189:LEU:CD2     | 19:4:203:LEU:CD2     | 2.64                     | 0.75              |
| 19:48:252:ARG:HG3    | 19:48:281:TRP:HH2    | 0.97                     | 0.75              |
| 19:48:293:LEU:HD13   | 19:48:316:PHE:CE1    | 2.21                     | 0.75              |
| 22:I16:171:MET:HE2   | 23:J16:592:VAL:HG13  | 1.65                     | 0.75              |
| 22:I16:335:SER:OG    | 23:J16:731:LEU:HD22  | 1.87                     | 0.75              |
| 10:C32:664:ASN:HA    | 10:C32:667:ILE:CG1   | 2.17                     | 0.75              |
| 1:R:1191:LYS:HD3     | 24:D:1453:GLU:OE1    | 1.84                     | 0.75              |
| 2:M:593:HIS:HD2      | 3:N:224:LEU:HD22     | 1.49                     | 0.75              |
| 1:R16:1168:LEU:HD23  | 1:R16:1216:ILE:HG13  | 1.66                     | 0.75              |
| 2:M16:416:VAL:HG11   | 8:L16:398:ALA:CB     | 2.14                     | 0.75              |
| 5:P:682:ARG:NH2      | 5:P:689:GLU:OE1      | 2.19                     | 0.75              |
| 8:L8:976:LEU:HD23    | 9:K8:1004:ARG:HD2    | 1.69                     | 0.75              |
| 9:K:1085:TYR:CE1     | 9:K:1093:SER:O       | 2.40                     | 0.75              |
| 9:K8:1198:LEU:CD1    | 9:K8:1267:LEU:CD2    | 2.65                     | 0.75              |
| 10:C16:1303:LEU:CD1  | 10:C16:1323:LEU:HD23 | 2.16                     | 0.75              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:1424:GLN:NE2  | 10:C24:1478:VAL:HG13 | 2.02                     | 0.75              |
| 10:C:1424:GLN:NE2    | 10:C:1478:VAL:HG13   | 2.02                     | 0.75              |
| 10:C8:1348:LEU:HD13  | 10:C8:1359:ILE:CG1   | 2.17                     | 0.75              |
| 11:A16:323:LEU:HD21  | 17:F8:74:ILE:HD12    | 1.67                     | 0.75              |
| 11:A16:468:VAL:O     | 11:A16:470:LEU:N     | 2.18                     | 0.75              |
| 17:F:71:GLU:C        | 17:F:73:GLY:N        | 2.42                     | 0.75              |
| 11:A32:354:ARG:HA    | 11:A32:452:TRP:CZ2   | 2.22                     | 0.75              |
| 11:A32:504:TYR:HB3   | 11:A32:505:PRO:HD3   | 1.69                     | 0.75              |
| 18:B:1112:LYS:CE     | 21:H:327:SER:CA      | 2.54                     | 0.75              |
| 18:B:1563:PHE:CZ     | 18:B:1567:ILE:HD11   | 2.22                     | 0.75              |
| 18:B:1618:HIS:CE1    | 18:B:1622:ILE:CD1    | 2.61                     | 0.75              |
| 18:B8:583:ARG:HH12   | 18:B8:711:CYS:HB2    | 1.46                     | 0.75              |
| 21:H:288:THR:CB      | 23:J32:650:GLN:HE21  | 1.98                     | 0.75              |
| 21:H8:312:GLN:HE22   | 22:I8:290:ASP:CB     | 1.99                     | 0.75              |
| 24:D40:839:GLU:CB    | 24:D40:971:HIS:CD2   | 2.70                     | 0.75              |
| 10:C32:847:ARG:NH2   | 10:C32:911:ILE:H     | 1.84                     | 0.75              |
| 10:C32:1541:PHE:CE1  | 10:C32:1649:LYS:HD2  | 2.19                     | 0.75              |
| 12:A48:798:PHE:HE1   | 12:A48:847:ARG:CZ    | 1.91                     | 0.75              |
| 1:R8:529:HIS:CE1     | 1:R8:529:HIS:NE2     | 2.55                     | 0.74              |
| 2:M16:816:ARG:HH11   | 2:M16:850:TYR:N      | 1.85                     | 0.74              |
| 4:T8:160:HIS:NE2     | 4:T8:160:HIS:CE1     | 2.55                     | 0.74              |
| 5:P:467:GLN:NE2      | 6:O:291:SER:CB       | 2.49                     | 0.74              |
| 7:Q:98:MET:HE2       | 7:Q:110:VAL:HG11     | 1.67                     | 0.74              |
| 5:P8:467:GLN:NE2     | 6:O8:291:SER:CB      | 2.49                     | 0.74              |
| 5:P16:394:ASN:C      | 5:P16:396:SER:N      | 2.44                     | 0.74              |
| 5:P16:682:ARG:NH2    | 5:P16:689:GLU:OE1    | 2.19                     | 0.74              |
| 10:C16:1333:HIS:HE1  | 10:C16:1337:LEU:HD23 | 1.51                     | 0.74              |
| 10:C24:1624:LEU:CD2  | 10:C24:1628:SER:HB2  | 2.16                     | 0.74              |
| 13:V:818:THR:CA      | 13:V:824:TRP:HE1     | 1.98                     | 0.74              |
| 19:48:189:LEU:CD2    | 19:48:203:LEU:CD2    | 2.64                     | 0.74              |
| 21:H8:194:VAL:HG13   | 21:H8:199:ASP:HB3    | 1.69                     | 0.74              |
| 22:I8:290:ASP:OD1    | 22:I8:293:LYS:CD     | 2.35                     | 0.74              |
| 24:D32:1109:LEU:HD22 | 24:D32:1156:SER:CB   | 2.14                     | 0.74              |
| 10:C32:1282:CYS:HA   | 10:C32:1738:MET:HE1  | 1.67                     | 0.74              |
| 2:M8:833:GLU:HG3     | 2:M8:836:ARG:HH21    | 1.51                     | 0.74              |
| 9:K:975:MET:HE1      | 9:K:1005:LEU:HD23    | 1.69                     | 0.74              |
| 10:C16:1340:PRO:HG2  | 10:C16:1746:GLY:HA3  | 1.69                     | 0.74              |
| 10:C16:1385:LEU:HB3  | 10:C16:1426:ARG:HH12 | 1.50                     | 0.74              |
| 11:A24:629:LEU:C     | 11:A24:678:LYS:HZ3   | 1.94                     | 0.74              |
| 10:C24:1303:LEU:HD13 | 10:C24:1323:LEU:CD2  | 2.16                     | 0.74              |
| 11:A40:603:ALA:HB1   | 11:A40:616:ARG:HD2   | 1.67                     | 0.74              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 13:V:814:MET:O      | 13:V:818:THR:OG1     | 2.03                     | 0.74              |
| 14:W:130:VAL:HG23   | 14:W:151:ILE:HD11    | 1.68                     | 0.74              |
| 10:C:847:ARG:NH2    | 10:C:911:ILE:H       | 1.84                     | 0.74              |
| 10:C:1340:PRO:HG2   | 10:C:1746:GLY:HA3    | 1.69                     | 0.74              |
| 10:C:1615:PHE:CB    | 10:C:1674:LEU:HD23   | 2.17                     | 0.74              |
| 18:B:536:ILE:HG23   | 18:B:545:VAL:HG12    | 1.68                     | 0.74              |
| 18:B:1900:ILE:HD11  | 18:B:1946:LEU:HD22   | 1.67                     | 0.74              |
| 18:B8:1575:GLN:HE21 | 24:D32:1403:LEU:HD23 | 0.62                     | 0.74              |
| 19:4:293:LEU:HD13   | 19:4:316:PHE:CE1     | 2.21                     | 0.74              |
| 22:I16:290:ASP:OD1  | 22:I16:293:LYS:CD    | 2.35                     | 0.74              |
| 24:D32:274:MET:HE3  | 24:D32:321:SER:HB2   | 1.69                     | 0.74              |
| 1:R:529:HIS:CE1     | 1:R:529:HIS:NE2      | 2.55                     | 0.74              |
| 3:N:208:LYS:HB3     | 3:N:239:ILE:HD13     | 1.69                     | 0.74              |
| 2:M8:537:ILE:HG13   | 2:M8:558:MET:HE3     | 1.69                     | 0.74              |
| 2:M8:641:CYS:HA     | 2:M8:644:TRP:NE1     | 2.02                     | 0.74              |
| 2:M16:403:LEU:HD21  | 2:M16:425:ALA:HB3    | 1.67                     | 0.74              |
| 5:P16:159:ILE:HD11  | 5:P16:214:LEU:HB3    | 1.69                     | 0.74              |
| 8:L16:1041:SER:OG   | 8:L16:1054:HIS:CE1   | 2.39                     | 0.74              |
| 10:C16:225:LEU:HD21 | 10:C16:388:TYR:OH    | 1.87                     | 0.74              |
| 10:C16:1278:ASP:OD2 | 21:H:283:LYS:HG2     | 1.87                     | 0.74              |
| 10:C16:1424:GLN:NE2 | 10:C16:1478:VAL:HG13 | 2.02                     | 0.74              |
| 11:A24:246:SER:OG   | 11:A24:500:ASP:OD2   | 2.02                     | 0.74              |
| 11:A40:587:VAL:HG21 | 11:A40:636:PHE:HE1   | 1.51                     | 0.74              |
| 11:A40:785:HIS:HB2  | 11:A40:793:ALA:HB2   | 1.69                     | 0.74              |
| 13:V:902:MET:HE1    | 14:W:777:LEU:CG      | 2.17                     | 0.74              |
| 10:C8:168:ARG:NH2   | 10:C8:227:ASP:O      | 2.21                     | 0.74              |
| 10:C8:1045:GLN:O    | 10:C8:1049:SER:OG    | 2.05                     | 0.74              |
| 10:C8:1358:ASP:HB3  | 10:C8:1361:LYS:HB2   | 1.67                     | 0.74              |
| 10:C8:1615:PHE:CB   | 10:C8:1674:LEU:HD23  | 2.17                     | 0.74              |
| 11:A32:785:HIS:HB2  | 11:A32:793:ALA:HB2   | 1.69                     | 0.74              |
| 18:B8:750:GLU:CD    | 18:B8:760:ARG:NH2    | 2.44                     | 0.74              |
| 20:E:37:LEU:HD13    | 20:E:222:ALA:HB1     | 1.70                     | 0.74              |
| 20:E8:8:GLU:HA      | 20:E8:278:GLU:OE1    | 1.87                     | 0.74              |
| 20:E8:432:ILE:HG21  | 24:D40:72:GLU:HG2    | 1.69                     | 0.74              |
| 10:C32:453:LEU:HB2  | 10:C32:486:LEU:HD23  | 1.67                     | 0.74              |
| 10:C32:1290:HIS:CG  | 10:C32:1334:MET:CE   | 2.70                     | 0.74              |
| 10:C32:1328:PHE:CZ  | 10:C32:1377:ILE:HD11 | 2.18                     | 0.74              |
| 2:M:420:CYS:HB3     | 8:L:391:TRP:CZ3      | 2.22                     | 0.74              |
| 2:M:833:GLU:HG3     | 2:M:836:ARG:HH21     | 1.51                     | 0.74              |
| 2:M8:755:THR:C      | 2:M8:757:VAL:H       | 1.95                     | 0.74              |
| 3:N8:208:LYS:HB3    | 3:N8:239:ILE:HD13    | 1.69                     | 0.74              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M16:408:GLU:CD    | 8:L16:484:PRO:HG3   | 2.12                     | 0.74              |
| 2:M16:816:ARG:HH12  | 2:M16:849:LEU:CA    | 1.99                     | 0.74              |
| 7:Q16:149:VAL:CG2   | 7:Q16:187:TRP:CZ2   | 2.70                     | 0.74              |
| 11:A24:43:LEU:HD23  | 23:J8:700:LEU:HD23  | 1.67                     | 0.74              |
| 11:A24:557:LEU:HD22 | 11:A24:561:ASP:HB3  | 1.67                     | 0.74              |
| 10:C24:1074:LEU:CD2 | 18:B8:256:VAL:O     | 2.35                     | 0.74              |
| 11:A40:20:LEU:CD1   | 21:H16:346:THR:HG23 | 2.18                     | 0.74              |
| 11:A40:743:ARG:HH22 | 24:D32:699:HIS:CD2  | 2.01                     | 0.74              |
| 12:A:388:VAL:H      | 12:A:459:ARG:HH11   | 1.33                     | 0.74              |
| 10:C:667:ILE:HG12   | 10:C:670:GLU:H      | 1.50                     | 0.74              |
| 10:C:1615:PHE:HB2   | 10:C:1674:LEU:CD2   | 2.16                     | 0.74              |
| 10:C8:1163:LEU:HD23 | 10:C8:1166:SER:HG   | 1.51                     | 0.74              |
| 11:A32:212:LYS:CE   | 11:A32:585:MET:HE3  | 2.14                     | 0.74              |
| 11:A32:323:LEU:HD21 | 17:F24:74:ILE:HD12  | 1.68                     | 0.74              |
| 18:B:1139:LYS:HB2   | 18:B:1365:ARG:NH1   | 2.02                     | 0.74              |
| 20:E8:434:TRP:NE1   | 24:D40:72:GLU:CD    | 2.30                     | 0.74              |
| 22:I:290:ASP:OD1    | 22:I:293:LYS:CD     | 2.36                     | 0.74              |
| 24:D8:274:MET:HE3   | 24:D8:321:SER:HB2   | 1.69                     | 0.74              |
| 10:C32:663:ILE:O    | 10:C32:667:ILE:HG23 | 1.87                     | 0.74              |
| 10:C32:717:GLU:O    | 10:C32:719:PRO:HD3  | 1.88                     | 0.74              |
| 10:C32:1541:PHE:HE1 | 10:C32:1649:LYS:HD2 | 1.50                     | 0.74              |
| 2:M8:417:ARG:HB3    | 8:L8:298:PHE:HE2    | 0.58                     | 0.74              |
| 3:N16:208:LYS:HB3   | 3:N16:239:ILE:HD13  | 1.69                     | 0.74              |
| 4:T:160:HIS:NE2     | 4:T:160:HIS:CE1     | 2.55                     | 0.74              |
| 4:T:386:HIS:NE2     | 4:T:386:HIS:CE1     | 2.56                     | 0.74              |
| 7:Q:219:GLY:HA2     | 7:Q:221:TRP:HE1     | 1.50                     | 0.74              |
| 7:Q16:98:MET:CE     | 7:Q16:110:VAL:HG11  | 2.16                     | 0.74              |
| 7:Q16:244:ILE:HG23  | 7:Q16:289:TYR:OH    | 1.85                     | 0.74              |
| 9:K8:1232:LEU:HD23  | 9:K8:1265:ILE:CG2   | 2.15                     | 0.74              |
| 10:C16:810:ASP:O    | 10:C16:814:SER:OG   | 2.05                     | 0.74              |
| 10:C16:966:CYS:HA   | 10:C16:1025:LEU:CD1 | 2.17                     | 0.74              |
| 11:A40:103:GLU:CG   | 21:H16:323:TYR:CE2  | 2.67                     | 0.74              |
| 11:A40:388:VAL:H    | 11:A40:459:ARG:HH11 | 1.33                     | 0.74              |
| 12:A:302:GLN:NE2    | 12:A:324:ARG:HH11   | 1.86                     | 0.74              |
| 10:C8:225:LEU:HD21  | 10:C8:388:TYR:OH    | 1.87                     | 0.74              |
| 11:A32:122:LYS:NZ   | 18:B8:1757:GLU:OE1  | 2.19                     | 0.74              |
| 11:A32:148:LEU:HD11 | 18:B8:1956:ILE:HD12 | 1.69                     | 0.74              |
| 18:B:437:PHE:CE1    | 18:B:473:LEU:HD13   | 2.23                     | 0.74              |
| 18:B8:437:PHE:CE1   | 18:B8:473:LEU:HD13  | 2.23                     | 0.74              |
| 18:B8:609:TYR:CE2   | 18:B8:610:VAL:HG22  | 2.22                     | 0.74              |
| 19:4:4:PHE:CD2      | 19:4:378:TYR:CE1    | 2.75                     | 0.74              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 19:4:187:SER:C       | 19:4:189:LEU:N       | 2.45                     | 0.74              |
| 19:4:295:SER:HB2     | 24:D24:224:ARG:HH21  | 1.51                     | 0.74              |
| 20:E8:49:THR:HA      | 20:E8:121:VAL:HG11   | 1.68                     | 0.74              |
| 21:H24:194:VAL:HG13  | 21:H24:199:ASP:HB3   | 1.69                     | 0.74              |
| 22:I24:203:GLN:CD    | 22:I24:209:TRP:CZ2   | 2.66                     | 0.74              |
| 21:H16:312:GLN:HE22  | 22:I16:290:ASP:CB    | 1.99                     | 0.74              |
| 22:I16:304:LEU:HB3   | 22:I16:305:PRO:HD3   | 1.68                     | 0.74              |
| 24:D:1013:HIS:NE2    | 24:D:1043:TYR:CD1    | 2.56                     | 0.74              |
| 10:C32:667:ILE:HD11  | 10:C32:700:MET:SD    | 2.27                     | 0.74              |
| 10:C32:966:CYS:HA    | 10:C32:1025:LEU:CD1  | 2.17                     | 0.74              |
| 12:A48:785:HIS:HB2   | 12:A48:793:ALA:HB2   | 1.69                     | 0.74              |
| 1:R16:529:HIS:CE1    | 1:R16:529:HIS:NE2    | 2.55                     | 0.74              |
| 6:O:38:SER:OG        | 6:O:40:THR:O         | 2.06                     | 0.74              |
| 9:K8:1085:TYR:CE1    | 9:K8:1093:SER:O      | 2.40                     | 0.74              |
| 10:C16:1328:PHE:CZ   | 10:C16:1377:ILE:HD11 | 2.18                     | 0.74              |
| 10:C24:1453:ARG:HH22 | 24:D24:1150:GLY:HA3  | 0.58                     | 0.74              |
| 11:A40:323:LEU:HD21  | 17:F16:74:ILE:HD12   | 1.68                     | 0.74              |
| 14:W:711:ARG:CZ      | 10:C8:1609:ASP:HB2   | 2.17                     | 0.74              |
| 10:C8:1010:ALA:N     | 10:C8:1192:ARG:HH21  | 1.81                     | 0.74              |
| 10:C8:1318:ARG:HD3   | 10:C8:1398:PHE:HD1   | 1.52                     | 0.74              |
| 11:A32:198:PRO:CB    | 11:A32:200:HIS:CE1   | 2.69                     | 0.74              |
| 19:4:250:ILE:HG12    | 20:E:165:ARG:NH2     | 2.00                     | 0.74              |
| 21:H8:288:THR:CB     | 23:J8:650:GLN:HE21   | 1.98                     | 0.74              |
| 24:D:274:MET:HE3     | 24:D:321:SER:HB2     | 1.69                     | 0.74              |
| 24:D40:274:MET:HE3   | 24:D40:321:SER:HB2   | 1.69                     | 0.74              |
| 2:M:626:PRO:HD2      | 3:N:165:GLY:C        | 2.11                     | 0.74              |
| 2:M:816:ARG:HH12     | 2:M:849:LEU:CA       | 2.00                     | 0.74              |
| 2:M8:627:TYR:CE2     | 3:N8:162:THR:HG21    | 2.22                     | 0.74              |
| 2:M16:626:PRO:HD2    | 3:N16:165:GLY:C      | 2.11                     | 0.74              |
| 5:P:134:SER:OG       | 5:P:176:GLU:OE2      | 2.06                     | 0.74              |
| 5:P8:105:ARG:NH1     | 5:P8:130:VAL:CG1     | 2.46                     | 0.74              |
| 9:K:1133:ILE:HD13    | 9:K:1152:PHE:CE2     | 2.23                     | 0.74              |
| 10:C16:1352:GLN:OE1  | 10:C16:1357:LEU:HD12 | 1.86                     | 0.74              |
| 10:C24:453:LEU:HD22  | 10:C24:459:LEU:HD22  | 1.60                     | 0.74              |
| 10:C24:966:CYS:HA    | 10:C24:1025:LEU:CD1  | 2.17                     | 0.74              |
| 10:C24:1340:PRO:HG2  | 10:C24:1746:GLY:HA3  | 1.69                     | 0.74              |
| 12:A:504:TYR:HB3     | 12:A:505:PRO:HD3     | 1.69                     | 0.74              |
| 13:V:844:MET:CG      | 10:C8:1502:ARG:HH22  | 1.74                     | 0.74              |
| 10:C:1290:HIS:CG     | 10:C:1334:MET:CE     | 2.70                     | 0.74              |
| 11:A32:471:ASN:C     | 11:A32:473:GLY:N     | 2.46                     | 0.74              |
| 18:B:583:ARG:HH12    | 18:B:711:CYS:HB2     | 1.46                     | 0.74              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 21:H:301:ARG:NH2     | 22:I:284:GLU:OE2     | 2.18                     | 0.74              |
| 24:D:1102:VAL:HG22   | 24:D:1153:GLN:CD     | 2.12                     | 0.74              |
| 10:C32:1615:PHE:CB   | 10:C32:1674:LEU:HD23 | 2.17                     | 0.74              |
| 2:M:641:CYS:HA       | 2:M:644:TRP:NE1      | 2.02                     | 0.74              |
| 2:M:755:THR:C        | 2:M:757:VAL:H        | 1.95                     | 0.74              |
| 2:M8:547:LYS:NZ      | 2:M8:554:PHE:HE1     | 1.85                     | 0.74              |
| 2:M8:627:TYR:CE2     | 3:N8:162:THR:CG2     | 2.71                     | 0.74              |
| 5:P:401:ARG:HD2      | 5:P:414:VAL:CB       | 2.18                     | 0.74              |
| 6:O8:38:SER:OG       | 6:O8:40:THR:O        | 2.06                     | 0.74              |
| 9:K:638:TRP:CE3      | 9:K:754:ARG:HD2      | 2.22                     | 0.74              |
| 9:K:788:LEU:O        | 9:K:792:LEU:HD23     | 1.88                     | 0.74              |
| 9:K:853:ALA:HB1      | 9:K:856:ILE:HD12     | 1.68                     | 0.74              |
| 9:K:975:MET:SD       | 9:K:1005:LEU:HD21    | 2.28                     | 0.74              |
| 9:K8:955:TYR:CD1     | 9:K8:985:PHE:HD2     | 2.06                     | 0.74              |
| 10:C24:1318:ARG:HD3  | 10:C24:1398:PHE:HD1  | 1.52                     | 0.74              |
| 11:A40:20:LEU:HD12   | 21:H16:346:THR:HG23  | 1.70                     | 0.74              |
| 10:C8:499:LEU:HD21   | 10:C8:505:PHE:CZ     | 2.23                     | 0.74              |
| 10:C8:1424:GLN:NE2   | 10:C8:1478:VAL:HG13  | 2.02                     | 0.74              |
| 11:A16:471:ASN:C     | 11:A16:473:GLY:N     | 2.46                     | 0.74              |
| 11:A16:785:HIS:HB2   | 11:A16:793:ALA:HB2   | 1.69                     | 0.74              |
| 18:B8:786:ASP:CG     | 24:D32:1066:VAL:CB   | 2.58                     | 0.74              |
| 18:B8:1139:LYS:HB2   | 18:B8:1365:ARG:NH1   | 2.03                     | 0.74              |
| 18:B8:1779:PRO:O     | 18:B8:1783:VAL:HG23  | 1.87                     | 0.74              |
| 20:E8:37:LEU:HD13    | 20:E8:222:ALA:HB1    | 1.69                     | 0.74              |
| 21:H:194:VAL:HG13    | 21:H:199:ASP:HB3     | 1.68                     | 0.74              |
| 21:H24:316:ILE:C     | 21:H24:318:ALA:N     | 2.45                     | 0.74              |
| 22:I24:335:SER:OG    | 23:J24:731:LEU:HD22  | 1.87                     | 0.74              |
| 21:H16:301:ARG:NH2   | 22:I16:284:GLU:OE2   | 2.18                     | 0.74              |
| 24:D24:1452:LYS:NZ   | 24:D32:971:HIS:NE2   | 2.35                     | 0.74              |
| 10:C32:810:ASP:O     | 10:C32:814:SER:OG    | 2.05                     | 0.74              |
| 10:C32:1348:LEU:HD13 | 10:C32:1359:ILE:CG1  | 2.18                     | 0.74              |
| 2:M8:540:TYR:HD1     | 2:M8:555:LEU:CD2     | 2.00                     | 0.74              |
| 2:M8:762:LEU:CG      | 2:M8:813:ASN:HD22    | 2.00                     | 0.74              |
| 2:M16:762:LEU:CB     | 2:M16:813:ASN:HD21   | 1.85                     | 0.74              |
| 5:P16:217:PHE:CE1    | 5:P16:221:LEU:CD1    | 2.71                     | 0.74              |
| 9:K:828:PRO:HB2      | 9:K:830:HIS:CE1      | 2.22                     | 0.74              |
| 9:K8:806:LEU:HD13    | 9:K8:874:VAL:CG1     | 2.18                     | 0.74              |
| 10:C16:717:GLU:O     | 10:C16:719:PRO:HD3   | 1.88                     | 0.74              |
| 11:A24:20:LEU:CD1    | 21:H8:346:THR:HG23   | 2.18                     | 0.74              |
| 10:C24:453:LEU:CD2   | 10:C24:459:LEU:CD1   | 2.66                     | 0.74              |
| 12:A:471:ASN:C       | 12:A:473:GLY:N       | 2.46                     | 0.74              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:V:808:LYS:HE3     | 15:J:616:ALA:HB1     | 1.68                     | 0.74              |
| 10:C:1686:LEU:HD23   | 10:C:1810:LEU:CD2    | 2.18                     | 0.74              |
| 10:C8:1303:LEU:CD1   | 10:C8:1323:LEU:HD23  | 2.16                     | 0.74              |
| 10:C8:1340:PRO:HG2   | 10:C8:1746:GLY:HA3   | 1.69                     | 0.74              |
| 11:A16:148:LEU:HD11  | 18:B:1956:ILE:HD12   | 1.69                     | 0.74              |
| 11:A16:198:PRO:CB    | 11:A16:200:HIS:CE1   | 2.69                     | 0.74              |
| 11:A32:468:VAL:C     | 11:A32:470:LEU:N     | 2.46                     | 0.74              |
| 18:B:603:PHE:CB      | 18:B:619:ARG:NH1     | 2.50                     | 0.74              |
| 18:B:1142:PHE:CE2    | 18:B:1348:VAL:HG11   | 2.23                     | 0.74              |
| 18:B8:86:LYS:NZ      | 18:B8:120:ALA:O      | 2.20                     | 0.74              |
| 18:B8:774:CYS:HB3    | 18:B8:788:LEU:HD11   | 1.70                     | 0.74              |
| 18:B8:1900:ILE:HD12  | 18:B8:1946:LEU:HD22  | 1.69                     | 0.74              |
| 20:E8:353:ILE:HB     | 20:E8:413:PHE:CE2    | 2.23                     | 0.74              |
| 22:I8:304:LEU:HB3    | 22:I8:305:PRO:HD3    | 1.68                     | 0.74              |
| 22:I24:290:ASP:OD1   | 22:I24:293:LYS:CD    | 2.36                     | 0.74              |
| 23:J24:718:GLN:CD    | 23:J24:737:TRP:HZ3   | 1.83                     | 0.74              |
| 21:H16:194:VAL:HG13  | 21:H16:199:ASP:HB3   | 1.69                     | 0.74              |
| 22:I16:203:GLN:CD    | 22:I16:209:TRP:CZ2   | 2.66                     | 0.74              |
| 10:C32:168:ARG:NH2   | 10:C32:227:ASP:O     | 2.21                     | 0.74              |
| 10:C32:225:LEU:HD21  | 10:C32:388:TYR:OH    | 1.87                     | 0.74              |
| 10:C32:225:LEU:HD21  | 10:C32:388:TYR:CZ    | 2.23                     | 0.74              |
| 1:R:1059:ILE:CG2     | 24:D:1435:ARG:NH2    | 2.51                     | 0.74              |
| 1:R8:634:ARG:HD3     | 4:T8:160:HIS:CE1     | 2.19                     | 0.74              |
| 1:R16:1349:ARG:HG3   | 1:R16:1390:GLU:HB3   | 1.70                     | 0.74              |
| 2:M16:816:ARG:CZ     | 2:M16:849:LEU:HB3    | 2.18                     | 0.74              |
| 2:M16:847:PHE:CB     | 4:T16:656:TRP:CH2    | 2.45                     | 0.74              |
| 10:C24:1439:ILE:HD13 | 10:C24:1457:LEU:HD13 | 1.70                     | 0.74              |
| 10:C24:1614:LEU:HD11 | 10:C24:1635:LEU:HD23 | 1.70                     | 0.74              |
| 13:V:832:LEU:CD2     | 13:V:836:LEU:HB3     | 2.18                     | 0.74              |
| 14:W:96:LYS:HE2      | 14:W:144:VAL:HG21    | 1.69                     | 0.74              |
| 10:C:390:HIS:CG      | 10:C:452:LEU:HB3     | 2.23                     | 0.74              |
| 10:C:1303:LEU:HD13   | 10:C:1323:LEU:CD2    | 2.16                     | 0.74              |
| 10:C8:1133:ILE:HG13  | 10:C8:1152:LYS:HZ2   | 1.53                     | 0.74              |
| 11:A16:122:LYS:NZ    | 18:B:1757:GLU:OE1    | 2.19                     | 0.74              |
| 11:A16:212:LYS:CE    | 11:A16:585:MET:HE3   | 2.14                     | 0.74              |
| 11:A16:706:SER:CB    | 24:D16:1398:ARG:CG   | 2.65                     | 0.74              |
| 18:B:1261:GLU:OE1    | 24:D16:1228:GLU:OE2  | 2.06                     | 0.74              |
| 18:B8:191:PHE:CE2    | 18:B8:193:LYS:CA     | 2.71                     | 0.74              |
| 18:B8:603:PHE:CB     | 18:B8:619:ARG:NH1    | 2.50                     | 0.74              |
| 18:B8:683:ASN:O      | 18:B8:685:SER:N      | 2.21                     | 0.74              |
| 18:B8:729:LEU:CD1    | 18:B8:1196:MET:CE    | 2.66                     | 0.74              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 19:48:178:ASN:OD1    | 20:E8:416:LYS:NZ     | 2.21                     | 0.74              |
| 20:E8:447:ILE:HG21   | 20:E8:451:ILE:HG22   | 1.70                     | 0.74              |
| 22:I:335:SER:OG      | 23:J32:731:LEU:HD22  | 1.87                     | 0.74              |
| 21:H24:301:ARG:NH2   | 22:I24:284:GLU:OE2   | 2.18                     | 0.74              |
| 24:D:400:VAL:CG2     | 24:D16:751:MET:HE2   | 2.17                     | 0.74              |
| 12:A48:587:VAL:HG21  | 12:A48:636:PHE:HE1   | 1.51                     | 0.74              |
| 2:M8:211:MET:HE3     | 3:N8:280:ASN:O       | 1.88                     | 0.73              |
| 2:M16:404:ASP:OD1    | 8:L16:390:LEU:HD11   | 1.87                     | 0.73              |
| 2:M16:641:CYS:HA     | 2:M16:644:TRP:NE1    | 2.02                     | 0.73              |
| 5:P:217:PHE:CE1      | 5:P:221:LEU:CD1      | 2.71                     | 0.73              |
| 10:C16:716:THR:HB    | 10:C16:717:GLU:OE1   | 1.88                     | 0.73              |
| 10:C16:1439:ILE:HD13 | 10:C16:1457:LEU:HD13 | 1.70                     | 0.73              |
| 11:A24:747:MET:SD    | 24:D16:167:ARG:NH2   | 2.55                     | 0.73              |
| 10:C24:1686:LEU:HD23 | 10:C24:1810:LEU:CD2  | 2.18                     | 0.73              |
| 10:C24:1688:ARG:HG2  | 23:J24:735:LYS:HE3   | 1.69                     | 0.73              |
| 11:A40:471:ASN:C     | 11:A40:473:GLY:N     | 2.46                     | 0.73              |
| 12:A:468:VAL:C       | 12:A:470:LEU:N       | 2.46                     | 0.73              |
| 13:V:794:ILE:CD1     | 15:J:599:LEU:HD22    | 2.06                     | 0.73              |
| 15:J:677:GLY:O       | 15:J:678:GLY:C       | 2.24                     | 0.73              |
| 10:C:168:ARG:NH2     | 10:C:227:ASP:O       | 2.21                     | 0.73              |
| 10:C:225:LEU:HD21    | 10:C:388:TYR:CZ      | 2.23                     | 0.73              |
| 10:C:499:LEU:HD21    | 10:C:505:PHE:CZ      | 2.23                     | 0.73              |
| 10:C:1318:ARG:HD3    | 10:C:1398:PHE:HD1    | 1.52                     | 0.73              |
| 10:C:1348:LEU:HD13   | 10:C:1359:ILE:CG1    | 2.18                     | 0.73              |
| 10:C8:1626:GLN:HE21  | 10:C8:1692:LYS:HZ3   | 1.32                     | 0.73              |
| 18:B:750:GLU:CD      | 18:B:760:ARG:NH2     | 2.45                     | 0.73              |
| 19:4:178:ASN:OD1     | 20:E:416:LYS:NZ      | 2.21                     | 0.73              |
| 19:4:306:ASP:OD1     | 19:4:307:PRO:HD2     | 1.88                     | 0.73              |
| 20:E:434:TRP:C       | 20:E:436:THR:H       | 1.96                     | 0.73              |
| 19:48:4:PHE:CD2      | 19:48:378:TYR:CE1    | 2.75                     | 0.73              |
| 22:I8:335:SER:OG     | 23:J8:731:LEU:HD22   | 1.87                     | 0.73              |
| 10:C32:1614:LEU:HD11 | 10:C32:1635:LEU:HD23 | 1.70                     | 0.73              |
| 12:A48:468:VAL:O     | 12:A48:470:LEU:N     | 2.18                     | 0.73              |
| 12:A48:504:TYR:HB3   | 12:A48:505:PRO:HD3   | 1.69                     | 0.73              |
| 1:R:983:ARG:CZ       | 24:D:1366:PRO:HD3    | 2.17                     | 0.73              |
| 1:R:1453:LYS:NZ      | 10:C:616:GLN:HG3     | 2.03                     | 0.73              |
| 2:M:211:MET:HE3      | 3:N:280:ASN:O        | 1.89                     | 0.73              |
| 2:M:468:HIS:HE1      | 2:M:511:LYS:O        | 1.71                     | 0.73              |
| 2:M8:185:ARG:HH12    | 2:M8:213:LEU:HD12    | 1.51                     | 0.73              |
| 5:P:16:PHE:HE2       | 5:P:461:HIS:HE1      | 1.34                     | 0.73              |
| 5:P:499:TYR:CE2      | 6:O:178:MET:SD       | 2.81                     | 0.73              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P8:217:PHE:CE1     | 5:P8:221:LEU:CD1     | 2.71                     | 0.73              |
| 5:P16:112:LEU:HD21   | 5:P16:122:TYR:CZ     | 2.11                     | 0.73              |
| 9:K:1198:LEU:CD1     | 9:K:1267:LEU:CD2     | 2.65                     | 0.73              |
| 9:K8:638:TRP:CE3     | 9:K8:754:ARG:HD2     | 2.22                     | 0.73              |
| 9:K8:840:TRP:HZ3     | 9:K8:907:ILE:HD12    | 1.48                     | 0.73              |
| 9:K8:1048:GLN:HE22   | 9:K8:1128:ARG:CG     | 2.01                     | 0.73              |
| 10:C16:1271:PHE:HE2  | 10:C16:1284:ASP:HB3  | 1.53                     | 0.73              |
| 11:A24:587:VAL:HG21  | 11:A24:636:PHE:HE1   | 1.52                     | 0.73              |
| 10:C24:499:LEU:HD21  | 10:C24:505:PHE:CZ    | 2.23                     | 0.73              |
| 10:C24:572:ILE:HD13  | 10:C24:606:MET:CE    | 2.18                     | 0.73              |
| 10:C24:1045:GLN:O    | 10:C24:1049:SER:OG   | 2.04                     | 0.73              |
| 10:C24:1290:HIS:HB2  | 10:C24:1334:MET:HE3  | 1.70                     | 0.73              |
| 13:V:796:HIS:NE2     | 13:V:800:LYS:HE3     | 2.04                     | 0.73              |
| 10:C:718:HIS:O       | 10:C:721:PHE:HB2     | 1.88                     | 0.73              |
| 11:A32:845:THR:OG1   | 24:D32:1297:HIS:HE1  | 1.69                     | 0.73              |
| 18:B8:1439:LYS:HZ1   | 24:D32:1257:ASN:CB   | 2.02                     | 0.73              |
| 20:E:473:LEU:CD1     | 20:E:514:PHE:HB3     | 2.18                     | 0.73              |
| 10:C32:345:MET:HE3   | 10:C32:401:ILE:HD11  | 1.46                     | 0.73              |
| 10:C32:1318:ARG:HD3  | 10:C32:1398:PHE:HD1  | 1.52                     | 0.73              |
| 10:C32:1424:GLN:NE2  | 10:C32:1478:VAL:HG13 | 2.02                     | 0.73              |
| 10:C32:1439:ILE:HD12 | 10:C32:1457:LEU:CD1  | 2.18                     | 0.73              |
| 12:A48:468:VAL:C     | 12:A48:470:LEU:N     | 2.46                     | 0.73              |
| 2:M:816:ARG:HH11     | 2:M:850:TYR:N        | 1.85                     | 0.73              |
| 2:M8:627:TYR:HE2     | 3:N8:162:THR:CB      | 2.02                     | 0.73              |
| 2:M16:231:ARG:CG     | 2:M16:299:GLY:CA     | 2.59                     | 0.73              |
| 5:P:322:CYS:CB       | 13:V:763:LYS:HE2     | 2.16                     | 0.73              |
| 5:P:607:PHE:CZ       | 5:P:633:LEU:CD1      | 2.71                     | 0.73              |
| 5:P8:159:ILE:HD11    | 5:P8:214:LEU:HB3     | 1.69                     | 0.73              |
| 5:P16:499:TYR:CE2    | 6:O16:178:MET:SD     | 2.81                     | 0.73              |
| 9:K:635:ALA:HB1      | 9:K:655:GLN:NE2      | 2.03                     | 0.73              |
| 10:C16:453:LEU:CD2   | 10:C16:459:LEU:CD1   | 2.66                     | 0.73              |
| 10:C16:572:ILE:HD13  | 10:C16:606:MET:HE2   | 1.70                     | 0.73              |
| 10:C16:1126:ASP:CG   | 24:D8:1069:GLY:HA3   | 2.12                     | 0.73              |
| 10:C16:1699:LYS:HZ2  | 23:J32:722:LEU:HD21  | 1.51                     | 0.73              |
| 11:A24:388:VAL:H     | 11:A24:459:ARG:HH11  | 1.33                     | 0.73              |
| 10:C24:565:ARG:HH11  | 10:C24:568:TRP:HB2   | 1.53                     | 0.73              |
| 11:A40:103:GLU:CD    | 21:H16:323:TYR:OH    | 2.30                     | 0.73              |
| 13:V:844:MET:HG2     | 10:C8:1502:ARG:HH21  | 0.91                     | 0.73              |
| 10:C8:1303:LEU:HD13  | 10:C8:1323:LEU:CD2   | 2.17                     | 0.73              |
| 10:C8:1686:LEU:HD23  | 10:C8:1810:LEU:CD2   | 2.18                     | 0.73              |
| 11:A16:20:LEU:CD1    | 21:H:346:THR:HG23    | 2.18                     | 0.73              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B8:1142:PHE:CE2   | 18:B8:1348:VAL:HG11 | 2.23                     | 0.73              |
| 18:B8:1768:ILE:CG2   | 18:B8:1770:THR:CG2  | 2.64                     | 0.73              |
| 20:E:447:ILE:HG21    | 20:E:451:ILE:HG22   | 1.69                     | 0.73              |
| 2:M:672:TYR:HB2      | 2:M:680:LYS:CD      | 2.18                     | 0.73              |
| 1:R8:1349:ARG:HG3    | 1:R8:1390:GLU:HB3   | 1.70                     | 0.73              |
| 2:M8:847:PHE:HB3     | 4:T8:656:TRP:CZ3    | 2.14                     | 0.73              |
| 2:M16:408:GLU:OE1    | 8:L16:484:PRO:HG2   | 1.88                     | 0.73              |
| 4:T16:386:HIS:NE2    | 4:T16:386:HIS:CE1   | 2.56                     | 0.73              |
| 5:P:12:GLU:O         | 5:P:14:VAL:N        | 2.19                     | 0.73              |
| 6:O8:103:MET:HE1     | 6:O8:124:MET:HE1    | 1.70                     | 0.73              |
| 9:K:1071:PHE:CE2     | 9:K:1107:LEU:HD23   | 2.24                     | 0.73              |
| 10:C16:572:ILE:HD13  | 10:C16:606:MET:CE   | 2.18                     | 0.73              |
| 10:C16:718:HIS:O     | 10:C16:721:PHE:HB2  | 1.88                     | 0.73              |
| 10:C16:1348:LEU:HD13 | 10:C16:1359:ILE:CG1 | 2.17                     | 0.73              |
| 10:C24:168:ARG:NH2   | 10:C24:227:ASP:O    | 2.21                     | 0.73              |
| 10:C:717:GLU:O       | 10:C:719:PRO:HD3    | 1.88                     | 0.73              |
| 10:C:1614:LEU:HD11   | 10:C:1635:LEU:HD23  | 1.70                     | 0.73              |
| 18:B:191:PHE:CE2     | 18:B:193:LYS:CA     | 2.71                     | 0.73              |
| 18:B:683:ASN:O       | 18:B:685:SER:N      | 2.21                     | 0.73              |
| 18:B:1768:ILE:CG2    | 18:B:1770:THR:CG2   | 2.64                     | 0.73              |
| 20:E:85:LEU:O        | 20:E:89:LEU:HD12    | 1.88                     | 0.73              |
| 19:48:306:ASP:OD1    | 19:48:307:PRO:HD2   | 1.88                     | 0.73              |
| 20:E8:319:ARG:HB3    | 20:E8:320:PRO:HD3   | 1.70                     | 0.73              |
| 1:R:1242:SER:OG      | 1:R:1244:LEU:HD12   | 1.89                     | 0.73              |
| 1:R16:1242:SER:OG    | 1:R16:1244:LEU:HD12 | 1.89                     | 0.73              |
| 4:T8:386:HIS:CE1     | 4:T8:386:HIS:NE2    | 2.56                     | 0.73              |
| 5:P:251:LYS:NZ       | 14:W:765:LYS:NZ     | 2.31                     | 0.73              |
| 5:P8:188:LEU:CD2     | 5:P8:380:MET:HE1    | 2.16                     | 0.73              |
| 5:P16:607:PHE:CB     | 5:P16:629:ARG:NH1   | 2.51                     | 0.73              |
| 7:Q16:183:ARG:NH1    | 7:Q16:231:HIS:CE1   | 2.57                     | 0.73              |
| 9:K8:1133:ILE:HD13   | 9:K8:1152:PHE:CE2   | 2.23                     | 0.73              |
| 10:C16:499:LEU:HD21  | 10:C16:505:PHE:CZ   | 2.23                     | 0.73              |
| 11:A24:20:LEU:HD12   | 21:H8:346:THR:HG23  | 1.70                     | 0.73              |
| 11:A40:468:VAL:C     | 11:A40:470:LEU:N    | 2.46                     | 0.73              |
| 11:A40:471:ASN:ND2   | 24:D32:1149:VAL:HB  | 2.02                     | 0.73              |
| 10:C:1304:VAL:HG13   | 10:C:1384:ILE:HD11  | 1.71                     | 0.73              |
| 10:C8:1614:LEU:HD11  | 10:C8:1635:LEU:HD23 | 1.70                     | 0.73              |
| 11:A32:20:LEU:HD12   | 21:H24:346:THR:HG23 | 1.70                     | 0.73              |
| 18:B:774:CYS:HB3     | 18:B:788:LEU:HD11   | 1.70                     | 0.73              |
| 18:B:1649:SER:HA     | 18:B:1653:LEU:HD12  | 1.71                     | 0.73              |
| 22:I:203:GLN:CD      | 22:I:209:TRP:CZ2    | 2.67                     | 0.73              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D40:1284:ILE:HD13 | 24:D40:1329:VAL:HG21 | 1.70                     | 0.73              |
| 10:C32:499:LEU:HD21  | 10:C32:505:PHE:CZ    | 2.23                     | 0.73              |
| 10:C32:1340:PRO:HG2  | 10:C32:1746:GLY:HA3  | 1.69                     | 0.73              |
| 2:M:156:GLY:HA2      | 10:C:571:ASP:OD1     | 1.89                     | 0.73              |
| 2:M:417:ARG:HH11     | 8:L:299:ASP:HA       | 1.54                     | 0.73              |
| 2:M8:762:LEU:HB2     | 2:M8:813:ASN:HD21    | 0.90                     | 0.73              |
| 2:M16:762:LEU:CG     | 2:M16:813:ASN:HD22   | 2.00                     | 0.73              |
| 5:P8:499:TYR:CE2     | 6:O8:178:MET:SD      | 2.81                     | 0.73              |
| 6:O16:38:SER:OG      | 6:O16:40:THR:O       | 2.06                     | 0.73              |
| 9:K:649:MET:CG       | 9:K:704:ARG:NH2      | 2.52                     | 0.73              |
| 9:K:1048:GLN:HE22    | 9:K:1128:ARG:CG      | 2.01                     | 0.73              |
| 9:K:1232:LEU:HD23    | 9:K:1265:ILE:CG2     | 2.15                     | 0.73              |
| 9:K8:635:ALA:HB1     | 9:K8:655:GLN:NE2     | 2.03                     | 0.73              |
| 10:C16:758:GLN:HE21  | 10:C16:819:GLN:HG2   | 1.54                     | 0.73              |
| 10:C16:1045:GLN:O    | 10:C16:1049:SER:OG   | 2.05                     | 0.73              |
| 10:C16:1686:LEU:HD23 | 10:C16:1810:LEU:CD2  | 2.18                     | 0.73              |
| 15:J:722:LEU:HD13    | 10:C8:1623:ILE:CD1   | 2.18                     | 0.73              |
| 10:C:810:ASP:O       | 10:C:814:SER:OG      | 2.05                     | 0.73              |
| 10:C8:664:ASN:CA     | 10:C8:667:ILE:HG12   | 2.17                     | 0.73              |
| 11:A16:20:LEU:HD12   | 21:H:346:THR:HG23    | 1.70                     | 0.73              |
| 11:A32:20:LEU:CD1    | 21:H24:346:THR:HG23  | 2.18                     | 0.73              |
| 18:B:86:LYS:NZ       | 18:B:120:ALA:O       | 2.20                     | 0.73              |
| 18:B:615:GLU:O       | 18:B:617:ASP:N       | 2.18                     | 0.73              |
| 18:B:729:LEU:CD1     | 18:B:1196:MET:CE     | 2.66                     | 0.73              |
| 18:B8:603:PHE:HB3    | 18:B8:619:ARG:NH1    | 2.02                     | 0.73              |
| 18:B8:683:ASN:C      | 18:B8:685:SER:N      | 2.47                     | 0.73              |
| 18:B8:1222:TYR:OH    | 18:B8:1240:ASP:OD2   | 2.07                     | 0.73              |
| 19:48:187:SER:C      | 19:48:189:LEU:N      | 2.45                     | 0.73              |
| 21:H16:231:HIS:HD2   | 23:J16:596:GLN:HE21  | 0.74                     | 0.73              |
| 10:C32:962:PHE:HZ    | 10:C32:997:ILE:HD12  | 1.50                     | 0.73              |
| 2:M8:816:ARG:CZ      | 2:M8:849:LEU:HB3     | 2.18                     | 0.73              |
| 1:R16:1112:LYS:HD3   | 5:P16:712:PHE:CE1    | 2.22                     | 0.73              |
| 10:C16:565:ARG:HH11  | 10:C16:568:TRP:HB2   | 1.54                     | 0.73              |
| 10:C16:1614:LEU:HD11 | 10:C16:1635:LEU:HD23 | 1.70                     | 0.73              |
| 11:A24:471:ASN:C     | 11:A24:473:GLY:H     | 1.96                     | 0.73              |
| 11:A24:471:ASN:C     | 11:A24:473:GLY:N     | 2.46                     | 0.73              |
| 11:A24:785:HIS:HB2   | 11:A24:793:ALA:HB2   | 1.69                     | 0.73              |
| 10:C24:1615:PHE:HB2  | 10:C24:1674:LEU:HD23 | 1.71                     | 0.73              |
| 12:A:785:HIS:HB2     | 12:A:793:ALA:HB2     | 1.69                     | 0.73              |
| 13:V:818:THR:HG23    | 13:V:824:TRP:CE2     | 2.24                     | 0.73              |
| 10:C:407:LYS:CG      | 10:C:465:PHE:CZ      | 2.70                     | 0.73              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:1779:PRO:O      | 18:B:1783:VAL:HG23   | 1.87                     | 0.73              |
| 18:B8:1649:SER:HA    | 18:B8:1653:LEU:HD12  | 1.71                     | 0.73              |
| 20:E:319:ARG:HB3     | 20:E:320:PRO:HD3     | 1.70                     | 0.73              |
| 20:E8:438:SER:C      | 20:E8:440:VAL:H      | 1.96                     | 0.73              |
| 24:D24:274:MET:HE3   | 24:D24:321:SER:HB2   | 1.70                     | 0.73              |
| 10:C32:1304:VAL:HG13 | 10:C32:1384:ILE:HD11 | 1.71                     | 0.73              |
| 1:R:1349:ARG:HG3     | 1:R:1390:GLU:HB3     | 1.70                     | 0.73              |
| 1:R8:1139:ARG:NH2    | 1:R8:1161:LEU:HD11   | 2.02                     | 0.73              |
| 1:R8:1466:LYS:CB     | 6:O8:160:LEU:CD1     | 2.48                     | 0.73              |
| 1:R16:1442:THR:CG2   | 3:N16:13:ILE:CD1     | 2.67                     | 0.73              |
| 5:P:251:LYS:CE       | 14:W:765:LYS:HE2     | 2.12                     | 0.73              |
| 5:P8:134:SER:OG      | 5:P8:176:GLU:OE2     | 2.06                     | 0.73              |
| 5:P8:394:ASN:C       | 5:P8:396:SER:N       | 2.44                     | 0.73              |
| 5:P16:313:TRP:CZ2    | 5:P16:345:MET:HE3    | 2.13                     | 0.73              |
| 8:L8:598:LEU:HD21    | 8:L8:627:ARG:CZ      | 2.18                     | 0.73              |
| 9:K:806:LEU:HD13     | 9:K:874:VAL:CG1      | 2.18                     | 0.73              |
| 10:C16:1318:ARG:HD3  | 10:C16:1398:PHE:HD1  | 1.52                     | 0.73              |
| 10:C16:1615:PHE:HB2  | 10:C16:1674:LEU:HD23 | 1.71                     | 0.73              |
| 10:C24:717:GLU:O     | 10:C24:719:PRO:HD3   | 1.88                     | 0.73              |
| 10:C24:1547:LYS:HE2  | 24:D24:1405:GLY:H    | 1.51                     | 0.73              |
| 10:C:1290:HIS:HB2    | 10:C:1334:MET:HE3    | 1.70                     | 0.73              |
| 10:C8:394:SER:HB3    | 10:C8:458:VAL:HG21   | 1.69                     | 0.73              |
| 10:C8:553:LEU:CD2    | 10:C8:595:THR:CG2    | 2.67                     | 0.73              |
| 10:C8:1615:PHE:HB2   | 10:C8:1674:LEU:HD23  | 1.71                     | 0.73              |
| 11:A32:36:ASN:HD21   | 22:I24:293:LYS:HE2   | 1.51                     | 0.73              |
| 18:B:683:ASN:C       | 18:B:685:SER:N       | 2.47                     | 0.73              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:HD13   | 1.71                     | 0.73              |
| 21:H:231:HIS:HD2     | 23:J32:596:GLN:HE21  | 0.74                     | 0.73              |
| 21:H:316:ILE:C       | 21:H:318:ALA:N       | 2.45                     | 0.73              |
| 10:C32:389:LEU:HD21  | 10:C32:447:PHE:HE1   | 1.41                     | 0.73              |
| 10:C32:565:ARG:CZ    | 10:C32:602:VAL:HG13  | 2.19                     | 0.73              |
| 10:C32:718:HIS:O     | 10:C32:721:PHE:HB2   | 1.88                     | 0.73              |
| 12:A48:388:VAL:H     | 12:A48:459:ARG:HH11  | 1.33                     | 0.73              |
| 1:R:1191:LYS:CB      | 24:D:1453:GLU:OE1    | 2.36                     | 0.73              |
| 1:R8:1442:THR:CG2    | 3:N8:13:ILE:CD1      | 2.67                     | 0.73              |
| 3:N8:267:TRP:HH2     | 3:N8:294:TRP:CH2     | 2.07                     | 0.73              |
| 1:R16:1223:PHE:CZ    | 5:P16:676:GLN:CD     | 2.66                     | 0.73              |
| 8:L8:1074:ARG:HB3    | 9:K8:1089:LYS:CE     | 2.19                     | 0.73              |
| 8:L16:1071:LEU:HD11  | 9:K16:1284:MET:CG    | 2.18                     | 0.73              |
| 11:A24:437:LEU:HD11  | 11:A24:454:LYS:HZ3   | 1.54                     | 0.73              |
| 11:A24:468:VAL:C     | 11:A24:470:LEU:N     | 2.46                     | 0.73              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C24:758:GLN:HE21  | 10:C24:819:GLN:HG2  | 1.54                     | 0.73              |
| 10:C24:879:LEU:HD21  | 10:C24:944:MET:SD   | 2.29                     | 0.73              |
| 10:C:553:LEU:CD2     | 10:C:595:THR:CG2    | 2.67                     | 0.73              |
| 10:C:565:ARG:HH11    | 10:C:568:TRP:HB2    | 1.54                     | 0.73              |
| 10:C:758:GLN:HE21    | 10:C:819:GLN:HG2    | 1.54                     | 0.73              |
| 10:C:879:LEU:HD21    | 10:C:944:MET:SD     | 2.29                     | 0.73              |
| 10:C:1439:ILE:HD12   | 10:C:1457:LEU:CD1   | 2.18                     | 0.73              |
| 10:C8:1283:LEU:HD11  | 10:C8:1357:LEU:HD11 | 1.71                     | 0.73              |
| 10:C8:1439:ILE:HD12  | 10:C8:1457:LEU:CD1  | 2.18                     | 0.73              |
| 10:C8:1439:ILE:HD13  | 10:C8:1457:LEU:HD13 | 1.70                     | 0.73              |
| 18:B:1148:ILE:HG12   | 18:B:1371:VAL:HG22  | 1.71                     | 0.73              |
| 20:E:353:ILE:HB      | 20:E:413:PHE:CE2    | 2.23                     | 0.73              |
| 10:C32:1163:LEU:HD23 | 10:C32:1166:SER:HG  | 1.53                     | 0.73              |
| 12:A48:471:ASN:C     | 12:A48:473:GLY:N    | 2.46                     | 0.73              |
| 1:R:1442:THR:CG2     | 3:N:13:ILE:CD1      | 2.66                     | 0.73              |
| 5:P:401:ARG:HH22     | 5:P:404:ILE:CG2     | 2.00                     | 0.73              |
| 5:P8:112:LEU:CD1     | 5:P8:123:GLN:NE2    | 2.52                     | 0.73              |
| 5:P8:611:LEU:HA      | 5:P8:629:ARG:NH2    | 2.04                     | 0.73              |
| 8:L8:175:ARG:NH2     | 12:A48:138:GLU:OE1  | 2.22                     | 0.73              |
| 8:L16:1054:HIS:CE1   | 8:L16:1054:HIS:NE2  | 2.57                     | 0.73              |
| 9:K8:792:LEU:HG      | 9:K8:864:ILE:CD1    | 2.19                     | 0.73              |
| 10:C24:65:PRO:CG     | 10:C24:96:ARG:NH2   | 2.44                     | 0.73              |
| 10:C24:286:ILE:HG23  | 10:C24:292:PHE:CD1  | 2.24                     | 0.73              |
| 10:C24:553:LEU:CD2   | 10:C24:595:THR:CG2  | 2.67                     | 0.73              |
| 11:A40:36:ASN:HD22   | 22:I16:293:LYS:HZ1  | 1.34                     | 0.73              |
| 14:W:598:ILE:CG1     | 14:W:626:LEU:HD23   | 2.18                     | 0.73              |
| 10:C:225:LEU:HD21    | 10:C:388:TYR:OH     | 1.87                     | 0.73              |
| 10:C8:879:LEU:HD21   | 10:C8:944:MET:SD    | 2.29                     | 0.73              |
| 10:C8:1466:ARG:HH12  | 16:A8:127:SER:HB3   | 1.54                     | 0.73              |
| 20:E:438:SER:C       | 20:E:440:VAL:H      | 1.96                     | 0.73              |
| 20:E8:434:TRP:C      | 20:E8:436:THR:H     | 1.96                     | 0.73              |
| 20:E8:473:LEU:CD1    | 20:E8:514:PHE:HB3   | 2.18                     | 0.73              |
| 21:H24:244:ARG:NH2   | 22:I24:177:VAL:HG13 | 2.04                     | 0.73              |
| 1:R8:1165:MET:HE3    | 1:R8:1220:GLN:HG2   | 1.71                     | 0.72              |
| 5:P:157:SER:O        | 5:P:251:LYS:NZ      | 2.22                     | 0.72              |
| 7:Q8:183:ARG:NH1     | 7:Q8:231:HIS:CE1    | 2.57                     | 0.72              |
| 10:C16:225:LEU:HD21  | 10:C16:388:TYR:CZ   | 2.23                     | 0.72              |
| 10:C16:553:LEU:CD2   | 10:C16:595:THR:CG2  | 2.67                     | 0.72              |
| 10:C16:879:LEU:HD21  | 10:C16:944:MET:SD   | 2.29                     | 0.72              |
| 10:C24:225:LEU:HD21  | 10:C24:388:TYR:CZ   | 2.23                     | 0.72              |
| 12:A:153:ARG:HB2     | 10:C8:74:ASP:OD1    | 1.89                     | 0.72              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 13:V:791:GLN:HA      | 15:J:599:LEU:HD21   | 1.71                     | 0.72              |
| 10:C:878:ARG:HH21    | 10:C:885:VAL:HG23   | 1.49                     | 0.72              |
| 10:C:1283:LEU:HD11   | 10:C:1357:LEU:HD11  | 1.71                     | 0.72              |
| 11:A16:36:ASN:HD22   | 22:I:293:LYS:HZ1    | 1.37                     | 0.72              |
| 11:A16:66:LEU:HD13   | 22:I:323:GLU:OE2    | 1.89                     | 0.72              |
| 11:A16:302:GLN:NE2   | 11:A16:324:ARG:HH11 | 1.86                     | 0.72              |
| 18:B:1390:LEU:HD11   | 18:B:1404:LEU:HD11  | 1.71                     | 0.72              |
| 18:B:1700:LEU:HD11   | 18:B:1721:LEU:HD21  | 1.70                     | 0.72              |
| 18:B8:266:ARG:NH1    | 18:B8:383:PHE:HB3   | 2.04                     | 0.72              |
| 19:4:293:LEU:CD1     | 19:4:316:PHE:HE1    | 2.01                     | 0.72              |
| 20:E:358:GLY:CA      | 20:E:454:MET:SD     | 2.77                     | 0.72              |
| 19:48:293:LEU:CD1    | 19:48:316:PHE:HE1   | 2.01                     | 0.72              |
| 21:H8:231:HIS:HD2    | 23:J8:596:GLN:HE21  | 0.74                     | 0.72              |
| 21:H16:316:ILE:C     | 21:H16:318:ALA:N    | 2.45                     | 0.72              |
| 2:M16:665:HIS:O      | 2:M16:684:GLN:NE2   | 2.21                     | 0.72              |
| 5:P:322:CYS:SG       | 13:V:763:LYS:CD     | 2.76                     | 0.72              |
| 8:L8:1054:HIS:CE1    | 8:L8:1054:HIS:NE2   | 2.57                     | 0.72              |
| 10:C16:721:PHE:O     | 10:C16:725:LEU:HD12 | 1.89                     | 0.72              |
| 10:C16:1290:HIS:HB2  | 10:C16:1334:MET:HE3 | 1.70                     | 0.72              |
| 10:C24:390:HIS:CB    | 10:C24:452:LEU:CD2  | 2.64                     | 0.72              |
| 10:C24:1682:VAL:CG2  | 10:C24:1758:LEU:CD2 | 2.67                     | 0.72              |
| 10:C:1682:VAL:CG2    | 10:C:1758:LEU:CD2   | 2.67                     | 0.72              |
| 11:A16:468:VAL:C     | 11:A16:470:LEU:N    | 2.46                     | 0.72              |
| 11:A16:471:ASN:C     | 11:A16:473:GLY:H    | 1.97                     | 0.72              |
| 11:A16:698:LYS:HE3   | 24:D16:1392:MET:HG2 | 1.71                     | 0.72              |
| 18:B:583:ARG:NH1     | 18:B:643:MET:HE1    | 2.05                     | 0.72              |
| 18:B:985:ASP:O       | 18:B:986:ALA:C      | 2.24                     | 0.72              |
| 18:B8:1390:LEU:HD11  | 18:B8:1404:LEU:HD11 | 1.71                     | 0.72              |
| 18:B8:1700:LEU:HD11  | 18:B8:1721:LEU:HD21 | 1.70                     | 0.72              |
| 19:4:188:ALA:C       | 19:4:190:ARG:N      | 2.45                     | 0.72              |
| 10:C32:144:ASP:HB3   | 10:C32:147:LEU:HD12 | 1.71                     | 0.72              |
| 1:R:1369:LEU:HD11    | 6:O:211:ASN:CG      | 2.13                     | 0.72              |
| 2:M8:569:LEU:CD2     | 3:N8:287:LYS:HD2    | 2.20                     | 0.72              |
| 3:N16:221:ASN:OD1    | 3:N16:224:LEU:N     | 2.22                     | 0.72              |
| 7:Q16:166:GLU:OE2    | 7:Q16:169:ARG:CZ    | 2.38                     | 0.72              |
| 8:L16:1071:LEU:CG    | 9:K16:1284:MET:SD   | 2.77                     | 0.72              |
| 10:C16:144:ASP:HB3   | 10:C16:147:LEU:HD12 | 1.71                     | 0.72              |
| 10:C24:718:HIS:O     | 10:C24:721:PHE:HB2  | 1.87                     | 0.72              |
| 10:C24:1348:LEU:HD13 | 10:C24:1359:ILE:CG1 | 2.18                     | 0.72              |
| 11:A40:103:GLU:CD    | 21:H16:323:TYR:HE2  | 1.87                     | 0.72              |
| 10:C8:1009:GLN:HB3   | 10:C8:1192:ARG:CZ   | 2.19                     | 0.72              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A32:66:LEU:HD13   | 22:I24:323:GLU:OE2  | 1.89                     | 0.72              |
| 18:B:1529:GLU:OE2    | 24:D16:1415:LEU:CD2 | 2.37                     | 0.72              |
| 18:B8:127:PHE:CE1    | 18:B8:131:ILE:HD11  | 2.24                     | 0.72              |
| 18:B8:583:ARG:NH1    | 18:B8:643:MET:HE1   | 2.04                     | 0.72              |
| 18:B8:1148:ILE:HG12  | 18:B8:1371:VAL:HG22 | 1.71                     | 0.72              |
| 20:E:138:ARG:NH2     | 20:E:190:TYR:CD2    | 2.58                     | 0.72              |
| 20:E:438:SER:C       | 20:E:440:VAL:N      | 2.47                     | 0.72              |
| 20:E8:138:ARG:NH2    | 20:E8:190:TYR:CD2   | 2.58                     | 0.72              |
| 21:H16:316:ILE:C     | 21:H16:318:ALA:H    | 1.98                     | 0.72              |
| 24:D8:1284:ILE:HD13  | 24:D8:1329:VAL:HG21 | 1.70                     | 0.72              |
| 10:C32:390:HIS:ND1   | 10:C32:452:LEU:CG   | 2.52                     | 0.72              |
| 2:M:185:ARG:HH12     | 2:M:213:LEU:HD12    | 1.51                     | 0.72              |
| 2:M:254:LEU:CD2      | 2:M:283:ILE:CG1     | 2.67                     | 0.72              |
| 1:R8:1101:ARG:CD     | 24:D40:1459:LEU:O   | 2.35                     | 0.72              |
| 1:R8:1242:SER:OG     | 1:R8:1244:LEU:HD12  | 1.89                     | 0.72              |
| 2:M8:468:HIS:HE1     | 2:M8:511:LYS:O      | 1.71                     | 0.72              |
| 8:L16:1030:LEU:CD1   | 9:K16:1285:GLU:HB2  | 2.04                     | 0.72              |
| 10:C16:168:ARG:NH2   | 10:C16:227:ASP:O    | 2.21                     | 0.72              |
| 10:C16:1318:ARG:HH21 | 10:C16:1396:SER:HG  | 1.37                     | 0.72              |
| 10:C24:1290:HIS:NE2  | 10:C24:1334:MET:HA  | 2.04                     | 0.72              |
| 11:A40:66:LEU:HD13   | 22:I16:323:GLU:OE2  | 1.89                     | 0.72              |
| 14:W:518:GLU:HG3     | 14:W:605:ASN:HD21   | 1.55                     | 0.72              |
| 10:C8:225:LEU:HD21   | 10:C8:388:TYR:CZ    | 2.23                     | 0.72              |
| 10:C8:286:ILE:HG23   | 10:C8:292:PHE:CD1   | 2.24                     | 0.72              |
| 10:C8:1271:PHE:CZ    | 10:C8:1284:ASP:OD1  | 2.29                     | 0.72              |
| 11:A32:323:LEU:HD11  | 11:A32:347:GLN:OE1  | 1.90                     | 0.72              |
| 11:A32:471:ASN:C     | 11:A32:473:GLY:H    | 1.96                     | 0.72              |
| 11:A32:674:GLY:HA3   | 24:D32:1396:PRO:HG3 | 1.70                     | 0.72              |
| 11:A32:798:PHE:HE1   | 11:A32:847:ARG:CZ   | 1.91                     | 0.72              |
| 18:B8:1700:LEU:HD23  | 18:B8:1833:PHE:CD2  | 2.25                     | 0.72              |
| 18:B8:1768:ILE:HD12  | 18:B8:1775:PHE:CE1  | 2.24                     | 0.72              |
| 20:E8:85:LEU:O       | 20:E8:89:LEU:HD12   | 1.88                     | 0.72              |
| 20:E8:123:CYS:HG     | 20:E8:135:ILE:HD13  | 1.53                     | 0.72              |
| 21:H16:244:ARG:NH2   | 22:I16:177:VAL:HG13 | 2.04                     | 0.72              |
| 24:D16:274:MET:HE3   | 24:D16:321:SER:HB2  | 1.69                     | 0.72              |
| 10:C32:286:ILE:HG23  | 10:C32:292:PHE:CD1  | 2.24                     | 0.72              |
| 1:R:1165:MET:HE3     | 1:R:1220:GLN:HG2    | 1.70                     | 0.72              |
| 2:M:816:ARG:CZ       | 2:M:849:LEU:HB3     | 2.19                     | 0.72              |
| 5:P:322:CYS:HB3      | 13:V:767:GLU:CD     | 2.13                     | 0.72              |
| 5:P8:352:LEU:HD22    | 5:P8:365:SER:OG     | 1.90                     | 0.72              |
| 7:Q8:166:GLU:OE2     | 7:Q8:169:ARG:CZ     | 2.38                     | 0.72              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:105:ARG:HH22   | 5:P16:133:TYR:HD1    | 0.74                     | 0.72              |
| 7:Q16:124:PHE:HD1    | 7:Q16:125:TYR:CD2    | 2.03                     | 0.72              |
| 10:C16:1290:HIS:NE2  | 10:C16:1334:MET:HA   | 2.04                     | 0.72              |
| 10:C16:1439:ILE:HD12 | 10:C16:1457:LEU:CD1  | 2.18                     | 0.72              |
| 10:C24:144:ASP:HB3   | 10:C24:147:LEU:HD12  | 1.71                     | 0.72              |
| 11:A40:302:GLN:NE2   | 11:A40:324:ARG:HH11  | 1.86                     | 0.72              |
| 14:W:518:GLU:HG3     | 14:W:605:ASN:ND2     | 2.04                     | 0.72              |
| 10:C:1290:HIS:NE2    | 10:C:1334:MET:HA     | 2.04                     | 0.72              |
| 10:C8:144:ASP:HB3    | 10:C8:147:LEU:HD12   | 1.71                     | 0.72              |
| 10:C8:1682:VAL:CG2   | 10:C8:1758:LEU:CD2   | 2.67                     | 0.72              |
| 18:B:266:ARG:NH1     | 18:B:383:PHE:HB3     | 2.04                     | 0.72              |
| 18:B:1725:THR:CG2    | 18:B:1830:LEU:HD22   | 2.15                     | 0.72              |
| 18:B:1900:ILE:HD12   | 18:B:1946:LEU:HD22   | 1.69                     | 0.72              |
| 18:B8:846:SER:OG     | 18:B8:899:LYS:CE     | 2.37                     | 0.72              |
| 20:E8:438:SER:C      | 20:E8:440:VAL:N      | 2.47                     | 0.72              |
| 21:H:244:ARG:NH2     | 22:I:177:VAL:HG13    | 2.03                     | 0.72              |
| 10:C32:1290:HIS:NE2  | 10:C32:1334:MET:HA   | 2.04                     | 0.72              |
| 2:M:569:LEU:CD2      | 3:N:287:LYS:HD2      | 2.20                     | 0.72              |
| 2:M:569:LEU:HD23     | 3:N:287:LYS:HD2      | 1.72                     | 0.72              |
| 1:R8:1486:SER:HA     | 2:M8:177:VAL:HG23    | 1.69                     | 0.72              |
| 5:P16:134:SER:OG     | 5:P16:176:GLU:OE2    | 2.06                     | 0.72              |
| 9:K:994:TYR:HD2      | 9:K:1023:LEU:HD11    | 1.55                     | 0.72              |
| 9:K8:1071:PHE:CE2    | 9:K8:1107:LEU:HD23   | 2.24                     | 0.72              |
| 10:C16:286:ILE:HG23  | 10:C16:292:PHE:CE1   | 2.25                     | 0.72              |
| 10:C16:1682:VAL:CG2  | 10:C16:1758:LEU:CD2  | 2.67                     | 0.72              |
| 11:A24:66:LEU:HD13   | 22:I8:323:GLU:OE2    | 1.89                     | 0.72              |
| 10:C24:619:LEU:HB3   | 10:C24:620:PRO:CD    | 2.19                     | 0.72              |
| 11:A40:474:LEU:CD1   | 24:D32:1099:ARG:HH12 | 2.03                     | 0.72              |
| 10:C:721:PHE:O       | 10:C:725:LEU:HD12    | 1.89                     | 0.72              |
| 10:C:1724:VAL:HG22   | 10:C:1736:ILE:HD12   | 1.72                     | 0.72              |
| 10:C8:1687:GLU:CD    | 10:C8:1806:ARG:HH21  | 1.97                     | 0.72              |
| 11:A32:445:ASN:CG    | 17:F24:65:ARG:NH1    | 2.28                     | 0.72              |
| 19:48:153:ARG:HH21   | 20:E8:467:ILE:CD1    | 2.00                     | 0.72              |
| 24:D32:1284:ILE:HD13 | 24:D32:1329:VAL:HG21 | 1.70                     | 0.72              |
| 10:C32:553:LEU:CD2   | 10:C32:595:THR:CG2   | 2.67                     | 0.72              |
| 1:R:1078:SER:OG      | 5:P:713:LEU:CD2      | 2.38                     | 0.72              |
| 3:N:4:GLN:NE2        | 3:N:44:GLY:C         | 2.39                     | 0.72              |
| 3:N:221:ASN:OD1      | 3:N:224:LEU:N        | 2.22                     | 0.72              |
| 3:N:267:TRP:HH2      | 3:N:294:TRP:CH2      | 2.07                     | 0.72              |
| 5:P16:425:TRP:HD1    | 5:P16:465:TYR:HH     | 1.35                     | 0.72              |
| 8:L16:1041:SER:CB    | 8:L16:1054:HIS:HE1   | 1.92                     | 0.72              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 8:L16:1069:LEU:HD11  | 9:K16:1086:VAL:HG12  | 1.68                     | 0.72              |
| 9:K8:649:MET:CG      | 9:K8:704:ARG:NH2     | 2.52                     | 0.72              |
| 10:C16:565:ARG:CZ    | 10:C16:569:PHE:CD2   | 2.68                     | 0.72              |
| 10:C16:1708:ARG:HG3  | 10:C16:1730:ILE:HD12 | 1.72                     | 0.72              |
| 10:C16:1770:LEU:O    | 10:C16:1836:LYS:CE   | 2.38                     | 0.72              |
| 10:C24:1009:GLN:HB3  | 10:C24:1192:ARG:CZ   | 2.19                     | 0.72              |
| 10:C24:1439:ILE:HD12 | 10:C24:1457:LEU:CD1  | 2.18                     | 0.72              |
| 11:A40:52:LEU:CD2    | 11:A40:55:GLU:OE2    | 2.37                     | 0.72              |
| 14:W:701:LEU:CD2     | 15:J:624:ALA:HB1     | 2.18                     | 0.72              |
| 10:C:572:ILE:HD13    | 10:C:606:MET:CE      | 2.18                     | 0.72              |
| 10:C8:390:HIS:NE2    | 10:C8:459:LEU:CD1    | 2.53                     | 0.72              |
| 10:C8:848:CYS:CA     | 10:C8:906:ARG:HH22   | 1.97                     | 0.72              |
| 18:B8:176:GLU:OE2    | 18:B8:227:CYS:SG     | 2.44                     | 0.72              |
| 18:B8:744:TYR:O      | 18:B8:748:SER:OG     | 2.07                     | 0.72              |
| 18:B8:1161:LEU:HD11  | 18:B8:1403:ILE:HD13  | 1.71                     | 0.72              |
| 10:C32:1290:HIS:HB2  | 10:C32:1334:MET:HE3  | 1.70                     | 0.72              |
| 1:R:1033:LYS:HZ3     | 24:D:1432:THR:CG2    | 2.03                     | 0.72              |
| 2:M:408:GLU:OE1      | 8:L:484:PRO:HG3      | 1.90                     | 0.72              |
| 2:M:447:LEU:HD21     | 8:L:280:GLN:NE2      | 2.04                     | 0.72              |
| 1:R8:1124:TRP:HZ2    | 4:T8:669:PRO:HG3     | 1.52                     | 0.72              |
| 2:M8:569:LEU:HD23    | 3:N8:287:LYS:HD2     | 1.72                     | 0.72              |
| 2:M8:626:PRO:HD2     | 3:N8:165:GLY:C       | 2.11                     | 0.72              |
| 2:M8:739:TYR:CE1     | 2:M8:798:MET:HE1     | 2.25                     | 0.72              |
| 2:M16:569:LEU:CD2    | 3:N16:287:LYS:HD2    | 2.20                     | 0.72              |
| 2:M16:739:TYR:CE1    | 2:M16:798:MET:HE1    | 2.25                     | 0.72              |
| 7:Q:183:ARG:NH1      | 7:Q:231:HIS:CE1      | 2.57                     | 0.72              |
| 5:P8:267:ARG:NH2     | 5:P8:270:GLU:CD      | 2.45                     | 0.72              |
| 10:C16:286:ILE:HG23  | 10:C16:292:PHE:CD1   | 2.24                     | 0.72              |
| 10:C16:1687:GLU:CD   | 10:C16:1806:ARG:HH21 | 1.97                     | 0.72              |
| 11:A24:302:GLN:NE2   | 11:A24:324:ARG:HH11  | 1.85                     | 0.72              |
| 10:C24:721:PHE:O     | 10:C24:725:LEU:HD12  | 1.89                     | 0.72              |
| 10:C24:1318:ARG:HH21 | 10:C24:1396:SER:HG   | 1.37                     | 0.72              |
| 11:A40:607:ARG:HH22  | 24:D32:914:PHE:HD1   | 1.37                     | 0.72              |
| 10:C:345:MET:HE3     | 10:C:401:ILE:HD11    | 1.46                     | 0.72              |
| 10:C:1009:GLN:HB3    | 10:C:1192:ARG:CZ     | 2.19                     | 0.72              |
| 10:C:1328:PHE:HZ     | 10:C:1377:ILE:CD1    | 2.01                     | 0.72              |
| 10:C8:586:PRO:HD2    | 10:C8:650:ARG:HH11   | 1.54                     | 0.72              |
| 11:A16:120:ALA:HB1   | 18:B:1520:LEU:HD13   | 1.72                     | 0.72              |
| 11:A16:676:TYR:CZ    | 24:D16:1395:SER:HB2  | 2.17                     | 0.72              |
| 11:A16:711:ARG:HD3   | 24:D16:1398:ARG:HG2  | 1.71                     | 0.72              |
| 11:A32:120:ALA:HB1   | 18:B8:1520:LEU:HD13  | 1.72                     | 0.72              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:302:GLN:NE2   | 11:A32:324:ARG:HH11  | 1.86                     | 0.72              |
| 18:B:266:ARG:NH1     | 18:B:383:PHE:CG      | 2.57                     | 0.72              |
| 18:B:1911:LEU:HB2    | 18:B:1960:LEU:CD1    | 2.20                     | 0.72              |
| 22:I24:131:ARG:NE    | 23:J24:557:ARG:HH21  | 1.88                     | 0.72              |
| 24:D:1284:ILE:HD13   | 24:D:1329:VAL:HG21   | 1.70                     | 0.72              |
| 24:D16:1284:ILE:HD13 | 24:D16:1329:VAL:HG21 | 1.69                     | 0.72              |
| 10:C32:407:LYS:NZ    | 10:C32:465:PHE:CE2   | 2.53                     | 0.72              |
| 10:C32:879:LEU:HD21  | 10:C32:944:MET:SD    | 2.29                     | 0.72              |
| 12:A48:302:GLN:NE2   | 12:A48:324:ARG:HH11  | 1.86                     | 0.72              |
| 1:R:1424:LYS:HE2     | 6:O:130:ASP:OD2      | 1.89                     | 0.72              |
| 2:M:428:SER:HB3      | 8:L:355:SER:HG       | 1.38                     | 0.72              |
| 1:R8:1466:LYS:CG     | 6:O8:160:LEU:CD2     | 2.61                     | 0.72              |
| 2:M16:468:HIS:HE1    | 2:M16:511:LYS:O      | 1.71                     | 0.72              |
| 5:P8:105:ARG:HH11    | 5:P8:130:VAL:HG13    | 1.55                     | 0.72              |
| 6:O16:103:MET:HE1    | 6:O16:124:MET:HE1    | 1.70                     | 0.72              |
| 8:L:1089:MET:HG2     | 9:K:1000:SER:CB      | 2.20                     | 0.72              |
| 9:K8:950:LYS:CE      | 9:K8:977:GLU:HB3     | 2.20                     | 0.72              |
| 11:A24:52:LEU:CD2    | 11:A24:55:GLU:OE2    | 2.37                     | 0.72              |
| 11:A24:607:ARG:NH1   | 24:D16:914:PHE:HE1   | 1.88                     | 0.72              |
| 11:A40:471:ASN:C     | 11:A40:473:GLY:H     | 1.97                     | 0.72              |
| 12:A:212:LYS:NZ      | 12:A:585:MET:CE      | 2.53                     | 0.72              |
| 12:A:312:LEU:HD11    | 12:A:364:ILE:HD11    | 1.71                     | 0.72              |
| 13:V:832:LEU:HD23    | 13:V:836:LEU:HB3     | 1.72                     | 0.72              |
| 13:V:839:LYS:HZ2     | 15:J:652:GLU:HG2     | 1.54                     | 0.72              |
| 13:V:902:MET:CG      | 15:J:696:LEU:HD21    | 2.20                     | 0.72              |
| 14:W:715:ASP:CA      | 10:C8:1568:ARG:HH11  | 1.86                     | 0.72              |
| 10:C:144:ASP:HB3     | 10:C:147:LEU:HD12    | 1.71                     | 0.72              |
| 10:C:286:ILE:HG23    | 10:C:292:PHE:CD1     | 2.24                     | 0.72              |
| 10:C:1271:PHE:CZ     | 10:C:1284:ASP:OD1    | 2.29                     | 0.72              |
| 10:C8:1318:ARG:HH21  | 10:C8:1396:SER:HG    | 1.36                     | 0.72              |
| 10:C8:1328:PHE:HZ    | 10:C8:1377:ILE:CD1   | 2.02                     | 0.72              |
| 11:A32:707:LEU:CB    | 24:D32:1398:ARG:NH2  | 2.48                     | 0.72              |
| 18:B:1070:GLY:O      | 18:B:1327:ARG:NH2    | 2.23                     | 0.72              |
| 18:B8:615:GLU:O      | 18:B8:617:ASP:N      | 2.18                     | 0.72              |
| 18:B8:1911:LEU:HB2   | 18:B8:1960:LEU:CD1   | 2.20                     | 0.72              |
| 20:E:429:PRO:HG2     | 24:D:69:VAL:CG1      | 2.17                     | 0.72              |
| 24:D40:1109:LEU:HD13 | 24:D40:1127:ARG:CD   | 2.20                     | 0.72              |
| 10:C32:65:PRO:CG     | 10:C32:96:ARG:NH2    | 2.44                     | 0.72              |
| 10:C32:821:ILE:CD1   | 10:C32:861:ILE:HG21  | 2.20                     | 0.72              |
| 10:C32:1682:VAL:CG2  | 10:C32:1758:LEU:CD2  | 2.67                     | 0.72              |
| 10:C32:1686:LEU:HD23 | 10:C32:1810:LEU:CD2  | 2.18                     | 0.72              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M16:211:MET:HE3    | 3:N16:280:ASN:O      | 1.88                     | 0.72              |
| 9:K:743:ARG:HH12     | 9:K:772:TYR:HE1      | 0.72                     | 0.72              |
| 9:K8:1248:LEU:CD1    | 9:K8:1265:ILE:HD11   | 2.07                     | 0.72              |
| 10:C16:1814:LYS:HE2  | 23:J32:738:MET:HE2   | 1.70                     | 0.72              |
| 12:A:323:LEU:HD11    | 12:A:347:GLN:OE1     | 1.90                     | 0.72              |
| 10:C:286:ILE:HG23    | 10:C:292:PHE:CE1     | 2.25                     | 0.72              |
| 10:C8:1304:VAL:HG13  | 10:C8:1384:ILE:HD11  | 1.71                     | 0.72              |
| 18:B:127:PHE:CE1     | 18:B:131:ILE:HD11    | 2.24                     | 0.72              |
| 18:B8:1110:LEU:HD21  | 21:H24:326:GLY:N     | 2.01                     | 0.72              |
| 24:D:387:LEU:CB      | 24:D16:746:ALA:HB2   | 2.19                     | 0.72              |
| 10:C32:1328:PHE:HZ   | 10:C32:1377:ILE:CD1  | 2.01                     | 0.72              |
| 10:C32:1439:ILE:HD13 | 10:C32:1457:LEU:HD13 | 1.70                     | 0.72              |
| 12:A48:471:ASN:C     | 12:A48:473:GLY:H     | 1.96                     | 0.72              |
| 1:R:526:ASN:CA       | 1:R:529:HIS:CE1      | 2.71                     | 0.71              |
| 2:M:246:ALA:C        | 2:M:290:ILE:HD13     | 2.14                     | 0.71              |
| 2:M:739:TYR:CE1      | 2:M:798:MET:HE1      | 2.25                     | 0.71              |
| 6:O:103:MET:HE1      | 6:O:124:MET:HE1      | 1.70                     | 0.71              |
| 8:L8:605:MET:HE2     | 8:L8:634:HIS:HD2     | 1.55                     | 0.71              |
| 9:K:584:SER:OG       | 9:K:622:VAL:CG2      | 2.34                     | 0.71              |
| 9:K:707:GLN:NE2      | 9:K:734:TRP:CE3      | 2.58                     | 0.71              |
| 9:K:950:LYS:CE       | 9:K:977:GLU:HB3      | 2.20                     | 0.71              |
| 10:C16:390:HIS:NE2   | 10:C16:449:GLU:HB2   | 2.03                     | 0.71              |
| 11:A24:390:ALA:HB1   | 24:D16:1099:ARG:CB   | 2.19                     | 0.71              |
| 11:A24:747:MET:HE1   | 24:D16:167:ARG:NH1   | 2.04                     | 0.71              |
| 10:C24:1133:ILE:HG13 | 10:C24:1152:LYS:NZ   | 2.05                     | 0.71              |
| 10:C24:1283:LEU:HD11 | 10:C24:1357:LEU:HD11 | 1.71                     | 0.71              |
| 10:C24:1304:VAL:HG13 | 10:C24:1384:ILE:HD11 | 1.71                     | 0.71              |
| 11:A40:803:PRO:HB3   | 24:D24:1401:LEU:HD12 | 0.74                     | 0.71              |
| 10:C:1615:PHE:HB2    | 10:C:1674:LEU:HD23   | 1.71                     | 0.71              |
| 10:C8:453:LEU:CD2    | 10:C8:459:LEU:CD1    | 2.66                     | 0.71              |
| 10:C8:619:LEU:HB3    | 10:C8:620:PRO:CD     | 2.19                     | 0.71              |
| 10:C8:639:MET:HE3    | 10:C8:643:LEU:HD11   | 1.71                     | 0.71              |
| 10:C8:821:ILE:CD1    | 10:C8:861:ILE:HG21   | 2.20                     | 0.71              |
| 10:C8:1724:VAL:HG22  | 10:C8:1736:ILE:HD12  | 1.72                     | 0.71              |
| 18:B8:266:ARG:NH1    | 18:B8:383:PHE:CG     | 2.57                     | 0.71              |
| 21:H8:244:ARG:NH2    | 22:I8:177:VAL:HG13   | 2.04                     | 0.71              |
| 21:H8:316:ILE:C      | 21:H8:318:ALA:H      | 1.98                     | 0.71              |
| 21:H24:231:HIS:HD2   | 23:J24:596:GLN:HE21  | 0.74                     | 0.71              |
| 22:I24:131:ARG:CG    | 23:J24:557:ARG:HH21  | 1.80                     | 0.71              |
| 24:D24:1284:ILE:HD13 | 24:D24:1329:VAL:HG21 | 1.70                     | 0.71              |
| 10:C32:721:PHE:O     | 10:C32:725:LEU:HD12  | 1.89                     | 0.71              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1687:GLU:CD   | 10:C32:1806:ARG:HH21 | 1.97                     | 0.71              |
| 5:P:352:LEU:HD22     | 5:P:365:SER:OG       | 1.90                     | 0.71              |
| 5:P:607:PHE:CZ       | 5:P:611:LEU:HD13     | 2.25                     | 0.71              |
| 5:P8:105:ARG:HH22    | 5:P8:130:VAL:HA      | 1.52                     | 0.71              |
| 7:Q8:149:VAL:HG23    | 7:Q8:187:TRP:CE2     | 2.26                     | 0.71              |
| 5:P16:547:PHE:HZ     | 7:Q16:227:SER:O      | 1.72                     | 0.71              |
| 9:K:735:ASP:OD2      | 9:K:794:ARG:NH2      | 2.24                     | 0.71              |
| 9:K:975:MET:HE1      | 9:K:1005:LEU:HD21    | 1.71                     | 0.71              |
| 9:K:1198:LEU:HD12    | 9:K:1267:LEU:CD2     | 2.20                     | 0.71              |
| 9:K8:707:GLN:NE2     | 9:K8:734:TRP:CE3     | 2.58                     | 0.71              |
| 9:K8:923:ILE:CG2     | 9:K8:929:ARG:HH21    | 2.02                     | 0.71              |
| 10:C16:761:VAL:HG22  | 10:C16:826:TYR:CD1   | 2.26                     | 0.71              |
| 10:C16:1133:ILE:HG13 | 10:C16:1152:LYS:NZ   | 2.05                     | 0.71              |
| 10:C24:553:LEU:HD22  | 10:C24:595:THR:CG2   | 2.19                     | 0.71              |
| 10:C24:1385:LEU:HB3  | 10:C24:1426:ARG:NH1  | 2.06                     | 0.71              |
| 11:A40:312:LEU:HD11  | 11:A40:364:ILE:HD11  | 1.71                     | 0.71              |
| 18:B:1152:ASP:CG     | 18:B:1378:LYS:HZ2    | 1.98                     | 0.71              |
| 18:B:1768:ILE:HD12   | 18:B:1775:PHE:CE1    | 2.24                     | 0.71              |
| 20:E:480:MET:HE2     | 20:E:493:TRP:CE3     | 2.24                     | 0.71              |
| 22:I:131:ARG:HG3     | 23:J32:557:ARG:HH22  | 1.46                     | 0.71              |
| 22:I8:131:ARG:HG3    | 23:J8:557:ARG:HH22   | 1.46                     | 0.71              |
| 24:D40:854:GLU:OE1   | 24:D40:927:GLN:OE1   | 2.08                     | 0.71              |
| 10:C32:1283:LEU:HD11 | 10:C32:1357:LEU:HD11 | 1.71                     | 0.71              |
| 10:C32:1770:LEU:O    | 10:C32:1836:LYS:CE   | 2.38                     | 0.71              |
| 2:M:345:ASP:C        | 2:M:347:LYS:N        | 2.31                     | 0.71              |
| 1:R8:1189:PRO:O      | 24:D40:1456:GLU:OE2  | 2.08                     | 0.71              |
| 2:M8:784:GLY:C       | 8:L16:472:GLU:OE2    | 2.33                     | 0.71              |
| 1:R16:526:ASN:CA     | 1:R16:529:HIS:CE1    | 2.71                     | 0.71              |
| 5:P8:614:VAL:H       | 5:P8:629:ARG:HH22    | 0.77                     | 0.71              |
| 9:K:923:ILE:CG2      | 9:K:929:ARG:HH21     | 2.02                     | 0.71              |
| 9:K8:743:ARG:HH12    | 9:K8:772:TYR:HE1     | 0.72                     | 0.71              |
| 9:K8:1117:LEU:HD11   | 9:K8:1135:THR:HG21   | 1.71                     | 0.71              |
| 11:A24:323:LEU:HD11  | 11:A24:347:GLN:OE1   | 1.90                     | 0.71              |
| 11:A24:465:SER:CB    | 24:D16:1100:GLN:HE22 | 1.94                     | 0.71              |
| 10:C24:286:ILE:HG23  | 10:C24:292:PHE:CE1   | 2.25                     | 0.71              |
| 10:C24:565:ARG:CZ    | 10:C24:569:PHE:CD2   | 2.67                     | 0.71              |
| 10:C24:1599:ASP:OD2  | 10:C24:1604:VAL:HB   | 1.91                     | 0.71              |
| 10:C24:1770:LEU:O    | 10:C24:1836:LYS:CE   | 2.38                     | 0.71              |
| 11:A40:323:LEU:HD11  | 11:A40:347:GLN:OE1   | 1.90                     | 0.71              |
| 10:C:572:ILE:HD13    | 10:C:606:MET:HE2     | 1.70                     | 0.71              |
| 10:C8:698:PHE:CE2    | 10:C8:749:LEU:HD11   | 2.25                     | 0.71              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A16:323:LEU:HD11  | 11:A16:347:GLN:OE1   | 1.90                     | 0.71              |
| 18:B8:643:MET:HE1    | 18:B8:711:CYS:CB     | 2.18                     | 0.71              |
| 18:B8:1070:GLY:O     | 18:B8:1327:ARG:NH2   | 2.23                     | 0.71              |
| 10:C32:1385:LEU:HB3  | 10:C32:1426:ARG:NH1  | 2.06                     | 0.71              |
| 2:M:672:TYR:CG       | 2:M:680:LYS:CD       | 2.73                     | 0.71              |
| 2:M8:401:ARG:HH22    | 8:L8:381:GLU:HB3     | 1.54                     | 0.71              |
| 2:M16:448:ASP:OD1    | 2:M16:448:ASP:N      | 2.21                     | 0.71              |
| 5:P16:603:LYS:O      | 5:P16:607:PHE:HD1    | 1.72                     | 0.71              |
| 7:Q16:149:VAL:HG23   | 7:Q16:187:TRP:CE2    | 2.26                     | 0.71              |
| 9:K8:1198:LEU:HD12   | 9:K8:1267:LEU:CD2    | 2.20                     | 0.71              |
| 11:A40:390:ALA:CB    | 24:D32:1099:ARG:CB   | 2.67                     | 0.71              |
| 11:A40:474:LEU:HD11  | 24:D32:1099:ARG:NH2  | 1.90                     | 0.71              |
| 14:W:706:LYS:HA      | 15:J:638:ASP:OD2     | 1.90                     | 0.71              |
| 10:C:821:ILE:CD1     | 10:C:861:ILE:HG21    | 2.20                     | 0.71              |
| 10:C8:1708:ARG:HG3   | 10:C8:1730:ILE:HD12  | 1.72                     | 0.71              |
| 11:A16:212:LYS:HE3   | 11:A16:585:MET:HE1   | 1.27                     | 0.71              |
| 22:I:131:ARG:NE      | 23:J32:557:ARG:HH21  | 1.88                     | 0.71              |
| 21:H24:316:ILE:C     | 21:H24:318:ALA:H     | 1.97                     | 0.71              |
| 10:C32:1061:ASN:O    | 10:C32:1062:GLU:C    | 2.25                     | 0.71              |
| 10:C32:1599:ASP:OD2  | 10:C32:1604:VAL:HB   | 1.91                     | 0.71              |
| 10:C32:1622:SER:OG   | 10:C32:1623:ILE:N    | 2.08                     | 0.71              |
| 10:C32:1724:VAL:HG22 | 10:C32:1736:ILE:HD12 | 1.72                     | 0.71              |
| 2:M8:762:LEU:CB      | 2:M8:813:ASN:HD21    | 1.85                     | 0.71              |
| 1:R16:1346:ILE:HD11  | 5:P16:685:PRO:HG2    | 1.71                     | 0.71              |
| 2:M16:628:LEU:CD1    | 3:N16:223:GLY:CA     | 2.68                     | 0.71              |
| 9:K8:735:ASP:OD2     | 9:K8:794:ARG:NH2     | 2.23                     | 0.71              |
| 9:K8:783:ARG:HB3     | 9:K8:785:ASP:OD1     | 1.91                     | 0.71              |
| 10:C16:586:PRO:HD2   | 10:C16:650:ARG:HH11  | 1.54                     | 0.71              |
| 10:C16:1304:VAL:HG13 | 10:C16:1384:ILE:HD11 | 1.71                     | 0.71              |
| 10:C16:1662:ASP:OD1  | 10:C24:1561:SER:OG   | 2.09                     | 0.71              |
| 10:C16:1724:VAL:HG22 | 10:C16:1736:ILE:HD12 | 1.72                     | 0.71              |
| 11:A24:212:LYS:NZ    | 11:A24:585:MET:CE    | 2.53                     | 0.71              |
| 11:A24:445:ASN:CG    | 17:F:65:ARG:NH1      | 2.28                     | 0.71              |
| 10:C24:1328:PHE:HZ   | 10:C24:1377:ILE:CD1  | 2.01                     | 0.71              |
| 10:C24:1708:ARG:HG3  | 10:C24:1730:ILE:HD12 | 1.72                     | 0.71              |
| 12:A:471:ASN:C       | 12:A:473:GLY:H       | 1.97                     | 0.71              |
| 12:A:707:LEU:HD11    | 12:A:767:ARG:HH12    | 1.55                     | 0.71              |
| 14:W:711:ARG:NH1     | 10:C8:1606:GLY:HA2   | 2.05                     | 0.71              |
| 10:C:280:SER:O       | 10:C:282:LYS:N       | 2.24                     | 0.71              |
| 10:C:452:LEU:HD12    | 10:C:453:LEU:N       | 2.04                     | 0.71              |
| 10:C:553:LEU:HD22    | 10:C:595:THR:CG2     | 2.19                     | 0.71              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:698:PHE:CE2     | 10:C:749:LEU:HD11    | 2.26                     | 0.71              |
| 10:C:1133:ILE:HG13   | 10:C:1152:LYS:NZ     | 2.05                     | 0.71              |
| 10:C:1439:ILE:HD13   | 10:C:1457:LEU:HD13   | 1.70                     | 0.71              |
| 10:C:1687:GLU:CD     | 10:C:1806:ARG:HH21   | 1.97                     | 0.71              |
| 10:C8:663:ILE:O      | 10:C8:667:ILE:HG23   | 1.90                     | 0.71              |
| 10:C8:1290:HIS:CG    | 10:C8:1334:MET:CE    | 2.70                     | 0.71              |
| 11:A32:112:ALA:CB    | 18:B8:1416:LYS:HZ1   | 2.02                     | 0.71              |
| 11:A32:212:LYS:NZ    | 11:A32:585:MET:CE    | 2.53                     | 0.71              |
| 11:A32:388:VAL:H     | 11:A32:459:ARG:HH11  | 1.33                     | 0.71              |
| 18:B:235:ARG:CZ      | 18:B:308:GLU:OE2     | 2.38                     | 0.71              |
| 18:B:782:THR:C       | 24:D16:1066:VAL:CG2  | 2.63                     | 0.71              |
| 18:B:846:SER:OG      | 18:B:899:LYS:CE      | 2.37                     | 0.71              |
| 18:B:1575:GLN:CD     | 24:D16:1403:LEU:HD23 | 2.14                     | 0.71              |
| 18:B8:235:ARG:CZ     | 18:B8:308:GLU:OE2    | 2.38                     | 0.71              |
| 18:B8:428:GLN:CG     | 18:B8:584:ARG:NH1    | 2.50                     | 0.71              |
| 18:B8:1152:ASP:CG    | 18:B8:1378:LYS:HZ2   | 1.98                     | 0.71              |
| 19:4:183:ARG:HH12    | 19:4:245:GLY:N       | 1.88                     | 0.71              |
| 20:E8:480:MET:HE2    | 20:E8:493:TRP:CE3    | 2.24                     | 0.71              |
| 21:H8:316:ILE:C      | 21:H8:318:ALA:N      | 2.45                     | 0.71              |
| 24:D:308:ASN:ND2     | 24:D16:753:ARG:CZ    | 2.52                     | 0.71              |
| 24:D:1009:CYS:C      | 24:D:1013:HIS:HD1    | 1.97                     | 0.71              |
| 10:C32:1466:ARG:HH12 | 12:A48:127:SER:HB3   | 1.54                     | 0.71              |
| 12:A48:312:LEU:HD11  | 12:A48:364:ILE:HD11  | 1.71                     | 0.71              |
| 1:R:1124:TRP:CH2     | 4:T:669:PRO:HG3      | 2.25                     | 0.71              |
| 2:M:624:ASP:O        | 3:N:165:GLY:CA       | 2.39                     | 0.71              |
| 2:M8:628:LEU:CD1     | 3:N8:223:GLY:CA      | 2.68                     | 0.71              |
| 7:Q:166:GLU:OE2      | 7:Q:169:ARG:CZ       | 2.38                     | 0.71              |
| 5:P8:607:PHE:CZ      | 5:P8:611:LEU:HD13    | 2.25                     | 0.71              |
| 8:L16:976:LEU:HD22   | 9:K16:1004:ARG:NE    | 1.98                     | 0.71              |
| 9:K8:584:SER:OG      | 9:K8:622:VAL:CG2     | 2.34                     | 0.71              |
| 9:K8:634:LEU:CD2     | 9:K8:754:ARG:HH12    | 2.00                     | 0.71              |
| 10:C16:619:LEU:HB3   | 10:C16:620:PRO:CD    | 2.19                     | 0.71              |
| 10:C24:1449:GLU:CD   | 24:D24:1151:SER:HA   | 2.15                     | 0.71              |
| 12:A:362:ARG:HG2     | 12:A:366:ARG:CZ      | 2.21                     | 0.71              |
| 14:W:586:ILE:CD1     | 15:J:572:ASP:OD2     | 2.38                     | 0.71              |
| 10:C:1166:SER:O      | 10:C:1168:PRO:N      | 2.24                     | 0.71              |
| 10:C8:1285:VAL:HG21  | 10:C8:1738:MET:HE3   | 1.61                     | 0.71              |
| 10:C8:1290:HIS:NE2   | 10:C8:1334:MET:HA    | 2.04                     | 0.71              |
| 11:A16:24:ALA:O      | 23:J32:705:TRP:NE1   | 2.23                     | 0.71              |
| 18:B:176:GLU:OE2     | 18:B:227:CYS:SG      | 2.44                     | 0.71              |
| 18:B:1419:LYS:HG3    | 18:B:1468:PHE:CZ     | 2.26                     | 0.71              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:1700:LEU:HD23  | 18:B:1833:PHE:CD2   | 2.24                     | 0.71              |
| 18:B8:1045:LYS:HZ3  | 18:B8:1100:LEU:HD23 | 1.54                     | 0.71              |
| 19:48:340:PRO:HD3   | 24:D8:140:ALA:CB    | 2.20                     | 0.71              |
| 21:H:316:ILE:C      | 21:H:318:ALA:H      | 1.98                     | 0.71              |
| 10:C32:553:LEU:HD22 | 10:C32:595:THR:CG2  | 2.19                     | 0.71              |
| 10:C32:667:ILE:HD11 | 10:C32:700:MET:CE   | 2.19                     | 0.71              |
| 2:M:328:THR:HG21    | 2:M:350:SER:CB      | 2.21                     | 0.71              |
| 1:R16:1124:TRP:CH2  | 4:T16:669:PRO:HG3   | 2.25                     | 0.71              |
| 5:P:377:LEU:HD12    | 14:W:23:PRO:HB3     | 1.71                     | 0.71              |
| 5:P8:547:PHE:HZ     | 7:Q8:227:SER:O      | 1.72                     | 0.71              |
| 8:L:1054:HIS:CE1    | 8:L:1054:HIS:NE2    | 2.57                     | 0.71              |
| 10:C16:278:ARG:HH11 | 10:C16:287:SER:HB2  | 1.56                     | 0.71              |
| 10:C16:553:LEU:HD22 | 10:C16:595:THR:CG2  | 2.19                     | 0.71              |
| 11:A24:24:ALA:O     | 23:J8:705:TRP:NE1   | 2.23                     | 0.71              |
| 11:A24:36:ASN:HD21  | 22:I8:293:LYS:HE2   | 1.52                     | 0.71              |
| 11:A40:787:ASP:OD1  | 11:A40:788:PRO:HD2  | 1.91                     | 0.71              |
| 13:V:835:GLU:HG3    | 15:J:648:TYR:OH     | 1.88                     | 0.71              |
| 10:C8:286:ILE:HG23  | 10:C8:292:PHE:CE1   | 2.25                     | 0.71              |
| 10:C8:553:LEU:HD22  | 10:C8:595:THR:CG2   | 2.19                     | 0.71              |
| 10:C8:1385:LEU:HB3  | 10:C8:1426:ARG:NH1  | 2.06                     | 0.71              |
| 10:C8:1770:LEU:O    | 10:C8:1836:LYS:CE   | 2.38                     | 0.71              |
| 11:A16:362:ARG:HG2  | 11:A16:366:ARG:CZ   | 2.21                     | 0.71              |
| 11:A32:36:ASN:HD22  | 22:I24:293:LYS:HZ1  | 1.38                     | 0.71              |
| 10:C32:280:SER:O    | 10:C32:282:LYS:N    | 2.24                     | 0.71              |
| 12:A48:323:LEU:HD11 | 12:A48:347:GLN:OE1  | 1.90                     | 0.71              |
| 2:M:210:GLN:NE2     | 10:C:529:GLN:HE21   | 1.88                     | 0.71              |
| 2:M:628:LEU:CD1     | 3:N:223:GLY:CA      | 2.68                     | 0.71              |
| 2:M8:651:ARG:HG3    | 2:M8:664:MET:HE1    | 1.73                     | 0.71              |
| 1:R16:1442:THR:CG2  | 3:N16:13:ILE:HD11   | 2.21                     | 0.71              |
| 3:N16:267:TRP:HH2   | 3:N16:294:TRP:CH2   | 2.07                     | 0.71              |
| 11:A24:468:VAL:HG21 | 24:D16:1100:GLN:CB  | 2.21                     | 0.71              |
| 13:V:902:MET:HE1    | 14:W:777:LEU:HD23   | 0.72                     | 0.71              |
| 10:C:52:SER:OG      | 24:D:1017:GLN:HG3   | 1.89                     | 0.71              |
| 11:A16:445:ASN:CG   | 17:F8:65:ARG:NH1    | 2.28                     | 0.71              |
| 11:A32:787:ASP:OD1  | 11:A32:788:PRO:HD2  | 1.91                     | 0.71              |
| 18:B:968:PHE:CB     | 18:B:1040:MET:HE2   | 2.20                     | 0.71              |
| 18:B:1739:LEU:HB3   | 18:B:1777:LEU:HD21  | 1.72                     | 0.71              |
| 18:B8:234:TRP:CD2   | 18:B8:309:MET:HE3   | 2.26                     | 0.71              |
| 18:B8:1739:LEU:HB3  | 18:B8:1777:LEU:HD21 | 1.72                     | 0.71              |
| 19:48:340:PRO:CD    | 24:D8:140:ALA:HB1   | 2.20                     | 0.71              |
| 24:D:308:ASN:CG     | 24:D16:753:ARG:HH21 | 1.97                     | 0.71              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 24:D32:1099:ARG:HG2 | 24:D32:1099:ARG:O   | 1.89                     | 0.71              |
| 10:C32:286:ILE:HG23 | 10:C32:292:PHE:CE1  | 2.25                     | 0.71              |
| 12:A48:362:ARG:HG2  | 12:A48:366:ARG:CZ   | 2.20                     | 0.71              |
| 1:R8:1124:TRP:CH2   | 4:T8:669:PRO:HG3    | 2.25                     | 0.71              |
| 2:M8:847:PHE:CB     | 4:T8:656:TRP:CH2    | 2.45                     | 0.71              |
| 5:P:325:PHE:CD2     | 13:V:771:GLN:NE2    | 2.58                     | 0.71              |
| 5:P:547:PHE:HZ      | 7:Q:227:SER:O       | 1.72                     | 0.71              |
| 5:P16:352:LEU:HD22  | 5:P16:365:SER:OG    | 1.90                     | 0.71              |
| 8:L:1096:GLU:CD     | 9:K:996:MET:HB3     | 2.15                     | 0.71              |
| 10:C16:1385:LEU:HB3 | 10:C16:1426:ARG:NH1 | 2.05                     | 0.71              |
| 10:C16:1691:GLU:OE2 | 23:J32:735:LYS:HA   | 1.90                     | 0.71              |
| 11:A24:312:LEU:HD11 | 11:A24:364:ILE:HD11 | 1.71                     | 0.71              |
| 10:C:453:LEU:CD2    | 10:C:459:LEU:CD1    | 2.66                     | 0.71              |
| 10:C:761:VAL:HG22   | 10:C:826:TYR:CD1    | 2.26                     | 0.71              |
| 10:C:1385:LEU:HB3   | 10:C:1426:ARG:NH1   | 2.05                     | 0.71              |
| 10:C:1708:ARG:HG3   | 10:C:1730:ILE:HD12  | 1.72                     | 0.71              |
| 10:C8:643:LEU:HD21  | 10:C8:656:THR:HG23  | 1.71                     | 0.71              |
| 10:C8:758:GLN:HE21  | 10:C8:819:GLN:HG2   | 1.54                     | 0.71              |
| 10:C8:1068:THR:O    | 10:C8:1069:TYR:C    | 2.25                     | 0.71              |
| 18:B:344:LYS:HE2    | 18:B:351:MET:HA     | 1.73                     | 0.71              |
| 18:B:428:GLN:CG     | 18:B:584:ARG:NH1    | 2.50                     | 0.71              |
| 18:B:643:MET:HE1    | 18:B:711:CYS:CB     | 2.18                     | 0.71              |
| 18:B:1291:LEU:HD12  | 18:B:1332:VAL:CG2   | 2.21                     | 0.71              |
| 24:D:405:GLN:OE1    | 24:D16:10:ARG:HD3   | 1.52                     | 0.71              |
| 1:R:1022:TYR:OH     | 24:D:1441:PRO:HB2   | 1.90                     | 0.71              |
| 1:R:1115:TYR:HB2    | 1:R:1131:MET:HE3    | 1.73                     | 0.71              |
| 1:R:1424:LYS:HD2    | 6:O:107:SER:OG      | 1.89                     | 0.71              |
| 1:R8:526:ASN:CA     | 1:R8:529:HIS:CE1    | 2.71                     | 0.71              |
| 1:R16:1165:MET:HE3  | 1:R16:1220:GLN:HG2  | 1.71                     | 0.71              |
| 2:M16:569:LEU:HD23  | 3:N16:287:LYS:HD2   | 1.72                     | 0.71              |
| 9:K:614:PHE:O       | 9:K:683:GLN:NE2     | 2.24                     | 0.71              |
| 10:C16:1009:GLN:HB3 | 10:C16:1192:ARG:CZ  | 2.20                     | 0.71              |
| 10:C24:1278:ASP:OD2 | 21:H24:283:LYS:CG   | 2.37                     | 0.71              |
| 10:C24:1699:LYS:HZ2 | 23:J24:722:LEU:HD21 | 1.55                     | 0.71              |
| 11:A40:212:LYS:NZ   | 11:A40:585:MET:CE   | 2.53                     | 0.71              |
| 12:A:437:LEU:HD11   | 12:A:454:LYS:HZ3    | 1.54                     | 0.71              |
| 10:C:168:ARG:HH11   | 10:C:229:PRO:HA     | 1.56                     | 0.71              |
| 10:C:1599:ASP:OD2   | 10:C:1604:VAL:HB    | 1.91                     | 0.71              |
| 10:C8:847:ARG:NE    | 10:C8:903:ASN:CG    | 2.49                     | 0.71              |
| 10:C8:1133:ILE:HG13 | 10:C8:1152:LYS:NZ   | 2.05                     | 0.71              |
| 10:C8:1599:ASP:OD2  | 10:C8:1604:VAL:HB   | 1.91                     | 0.71              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A16:312:LEU:HD11 | 11:A16:364:ILE:HD11  | 1.71                     | 0.71              |
| 18:B:744:TYR:O      | 18:B:748:SER:OG      | 2.07                     | 0.71              |
| 18:B:1802:ASP:C     | 18:B:1804:THR:H      | 1.99                     | 0.71              |
| 18:B8:968:PHE:CB    | 18:B8:1040:MET:HE2   | 2.20                     | 0.71              |
| 18:B8:1419:LYS:HG3  | 18:B8:1468:PHE:CZ    | 2.26                     | 0.71              |
| 21:H24:287:ILE:HG23 | 22:I24:273:LEU:HD11  | 1.73                     | 0.71              |
| 10:C32:761:VAL:HG22 | 10:C32:826:TYR:CD1   | 2.26                     | 0.71              |
| 1:R:1428:VAL:CG2    | 6:O:165:LYS:HE2      | 2.19                     | 0.70              |
| 2:M:254:LEU:CD2     | 2:M:283:ILE:CD1      | 2.68                     | 0.70              |
| 1:R8:1442:THR:CG2   | 3:N8:13:ILE:HD11     | 2.21                     | 0.70              |
| 2:M16:328:THR:HG21  | 2:M16:350:SER:CB     | 2.21                     | 0.70              |
| 9:K8:1110:GLN:O     | 9:K8:1114:THR:OG1    | 2.09                     | 0.70              |
| 10:C16:390:HIS:CG   | 10:C16:452:LEU:CB    | 2.66                     | 0.70              |
| 10:C16:407:LYS:NZ   | 10:C16:465:PHE:CE2   | 2.53                     | 0.70              |
| 10:C16:698:PHE:CE2  | 10:C16:749:LEU:HD11  | 2.26                     | 0.70              |
| 10:C16:1328:PHE:HZ  | 10:C16:1377:ILE:CD1  | 2.01                     | 0.70              |
| 10:C24:572:ILE:HD13 | 10:C24:606:MET:HE2   | 1.70                     | 0.70              |
| 11:A40:70:GLU:O     | 21:H16:351:ARG:NH1   | 2.24                     | 0.70              |
| 14:W:598:ILE:HG12   | 14:W:626:LEU:CD2     | 2.21                     | 0.70              |
| 11:A16:388:VAL:H    | 11:A16:459:ARG:HH11  | 1.33                     | 0.70              |
| 11:A32:362:ARG:HG2  | 11:A32:366:ARG:CZ    | 2.21                     | 0.70              |
| 18:B:583:ARG:NH2    | 18:B:711:CYS:HB2     | 2.06                     | 0.70              |
| 18:B8:344:LYS:HE2   | 18:B8:351:MET:HA     | 1.73                     | 0.70              |
| 18:B8:1802:ASP:C    | 18:B8:1804:THR:H     | 1.99                     | 0.70              |
| 20:E8:25:PRO:HG3    | 20:E8:237:ILE:HD11   | 1.72                     | 0.70              |
| 20:E8:73:ASP:OD1    | 20:E8:96:ARG:NH2     | 2.24                     | 0.70              |
| 21:H:287:ILE:HG23   | 22:I:273:LEU:HD11    | 1.73                     | 0.70              |
| 21:H8:338:MET:CE    | 23:J8:692:VAL:HG21   | 2.21                     | 0.70              |
| 22:I8:131:ARG:NE    | 23:J8:557:ARG:HH21   | 1.88                     | 0.70              |
| 21:H24:338:MET:CE   | 23:J24:692:VAL:HG21  | 2.21                     | 0.70              |
| 10:C32:698:PHE:CE2  | 10:C32:749:LEU:HD11  | 2.26                     | 0.70              |
| 10:C32:1009:GLN:HB3 | 10:C32:1192:ARG:CZ   | 2.20                     | 0.70              |
| 10:C32:1286:MET:HE3 | 10:C32:1344:VAL:HG11 | 1.73                     | 0.70              |
| 1:R:1078:SER:OG     | 5:P:713:LEU:HD23     | 1.91                     | 0.70              |
| 2:M:254:LEU:HD22    | 2:M:283:ILE:HD13     | 1.73                     | 0.70              |
| 2:M:819:GLN:OE1     | 2:M:846:LEU:HD21     | 1.91                     | 0.70              |
| 3:N:26:ILE:CD1      | 3:N:40:VAL:HG21      | 2.21                     | 0.70              |
| 2:M16:627:TYR:CE1   | 3:N16:162:THR:CG2    | 2.74                     | 0.70              |
| 2:M16:651:ARG:HG3   | 2:M16:664:MET:HE1    | 1.73                     | 0.70              |
| 3:N16:26:ILE:CD1    | 3:N16:40:VAL:HG21    | 2.21                     | 0.70              |
| 4:T16:671:ILE:HD12  | 5:P16:698:GLY:C      | 2.16                     | 0.70              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 5:P:401:ARG:HD2     | 5:P:414:VAL:HG11     | 1.72                     | 0.70              |
| 5:P8:16:PHE:HD1     | 6:O8:311:LEU:CD1     | 2.03                     | 0.70              |
| 5:P16:267:ARG:NH2   | 5:P16:270:GLU:CD     | 2.45                     | 0.70              |
| 9:K8:1154:TRP:CH2   | 9:K8:1219:VAL:HG13   | 2.26                     | 0.70              |
| 9:K8:1154:TRP:CE2   | 9:K8:1219:VAL:HG11   | 2.25                     | 0.70              |
| 10:C16:821:ILE:CD1  | 10:C16:861:ILE:HG21  | 2.20                     | 0.70              |
| 11:A24:225:ARG:HH11 | 11:A24:228:MET:HE1   | 1.56                     | 0.70              |
| 11:A24:362:ARG:HG2  | 11:A24:366:ARG:CZ    | 2.21                     | 0.70              |
| 11:A24:787:ASP:OD1  | 11:A24:788:PRO:HD2   | 1.91                     | 0.70              |
| 10:C24:1687:GLU:CD  | 10:C24:1806:ARG:HH21 | 1.97                     | 0.70              |
| 11:A40:36:ASN:HD21  | 22:I16:293:LYS:HE2   | 1.52                     | 0.70              |
| 11:A40:326:TYR:CD1  | 17:F16:77:TYR:HB3    | 2.13                     | 0.70              |
| 12:A:273:ARG:NH2    | 12:A:480:ASP:OD1     | 2.24                     | 0.70              |
| 12:A:468:VAL:C      | 12:A:470:LEU:H       | 1.99                     | 0.70              |
| 10:C:452:LEU:HD12   | 10:C:453:LEU:HG      | 1.73                     | 0.70              |
| 10:C:620:PRO:HB3    | 10:C:636:VAL:HG13    | 1.58                     | 0.70              |
| 10:C:979:MET:HE3    | 10:C:1028:ILE:HG22   | 0.72                     | 0.70              |
| 10:C:1318:ARG:HH21  | 10:C:1396:SER:HG     | 1.38                     | 0.70              |
| 11:A16:212:LYS:NZ   | 11:A16:585:MET:CE    | 2.53                     | 0.70              |
| 11:A32:24:ALA:O     | 23:J24:705:TRP:NE1   | 2.23                     | 0.70              |
| 18:B:1161:LEU:CD1   | 18:B:1403:ILE:CG2    | 2.68                     | 0.70              |
| 18:B:1563:PHE:CE1   | 18:B:1567:ILE:HD11   | 2.26                     | 0.70              |
| 18:B8:349:PHE:CZ    | 18:B8:353:ILE:CD1    | 2.58                     | 0.70              |
| 20:E8:432:ILE:HG21  | 24:D40:72:GLU:OE1    | 1.91                     | 0.70              |
| 10:C32:847:ARG:CZ   | 10:C32:903:ASN:CG    | 2.64                     | 0.70              |
| 10:C32:1166:SER:O   | 10:C32:1168:PRO:N    | 2.24                     | 0.70              |
| 10:C32:1615:PHE:HB2 | 10:C32:1674:LEU:HD23 | 1.71                     | 0.70              |
| 1:R:1442:THR:CG2    | 3:N:13:ILE:HD11      | 2.21                     | 0.70              |
| 2:M:417:ARG:CA      | 8:L:346:TRP:CZ2      | 2.73                     | 0.70              |
| 2:M8:351:ALA:CB     | 8:L8:219:ILE:HG23    | 2.21                     | 0.70              |
| 2:M8:624:ASP:O      | 3:N8:165:GLY:CA      | 2.39                     | 0.70              |
| 8:L8:1077:LEU:CD1   | 9:K8:1086:VAL:CG1    | 2.65                     | 0.70              |
| 9:K:1154:TRP:CH2    | 9:K:1219:VAL:HG13    | 2.26                     | 0.70              |
| 10:C16:847:ARG:NE   | 10:C16:903:ASN:CG    | 2.50                     | 0.70              |
| 10:C16:1699:LYS:NZ  | 23:J32:722:LEU:HD21  | 2.00                     | 0.70              |
| 10:C24:847:ARG:NE   | 10:C24:903:ASN:CG    | 2.49                     | 0.70              |
| 10:C24:1286:MET:HE3 | 10:C24:1344:VAL:HG11 | 1.73                     | 0.70              |
| 12:A:127:SER:HB3    | 10:C:1466:ARG:HH12   | 1.54                     | 0.70              |
| 10:C8:761:VAL:HG22  | 10:C8:826:TYR:CD1    | 2.26                     | 0.70              |
| 10:C8:922:ALA:HB1   | 10:C8:923:PRO:HD2    | 1.74                     | 0.70              |
| 10:C8:960:PHE:CZ    | 10:C8:1138:GLU:OE1   | 2.43                     | 0.70              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:711:ARG:HD3   | 24:D32:1398:ARG:CG   | 2.20                     | 0.70              |
| 21:H:291:VAL:CG1     | 23:J32:657:GLU:HG3   | 2.21                     | 0.70              |
| 21:H16:338:MET:CE    | 23:J16:692:VAL:HG21  | 2.21                     | 0.70              |
| 12:A48:212:LYS:NZ    | 12:A48:585:MET:CE    | 2.53                     | 0.70              |
| 1:R8:1466:LYS:HD2    | 6:O8:160:LEU:HD13    | 1.72                     | 0.70              |
| 2:M8:627:TYR:CE2     | 3:N8:162:THR:CB      | 2.75                     | 0.70              |
| 6:O:105:ASN:ND2      | 6:O:134:ARG:HH22     | 1.89                     | 0.70              |
| 7:Q16:295:SER:HB2    | 7:Q16:297:VAL:HG23   | 1.73                     | 0.70              |
| 8:L:346:TRP:CZ3      | 8:L:350:THR:CG2      | 2.74                     | 0.70              |
| 8:L16:1096:GLU:OE1   | 9:K16:998:GLN:HG3    | 1.89                     | 0.70              |
| 9:K:1117:LEU:HD11    | 9:K:1135:THR:HG21    | 1.71                     | 0.70              |
| 10:C16:1283:LEU:HD11 | 10:C16:1357:LEU:HD11 | 1.71                     | 0.70              |
| 10:C16:1466:ARG:HH12 | 11:A24:127:SER:HB3   | 1.54                     | 0.70              |
| 11:A24:70:GLU:O      | 21:H8:351:ARG:NH1    | 2.24                     | 0.70              |
| 10:C24:821:ILE:CD1   | 10:C24:861:ILE:HG21  | 2.20                     | 0.70              |
| 10:C24:1271:PHE:HE2  | 10:C24:1284:ASP:HB3  | 1.53                     | 0.70              |
| 13:V:814:MET:CE      | 13:V:824:TRP:HH2     | 2.04                     | 0.70              |
| 14:W:516:GLN:C       | 14:W:604:PRO:HB2     | 2.15                     | 0.70              |
| 10:C8:572:ILE:HD13   | 10:C8:606:MET:HE2    | 1.70                     | 0.70              |
| 11:A16:707:LEU:HD11  | 11:A16:767:ARG:HH12  | 1.55                     | 0.70              |
| 11:A32:225:ARG:HH11  | 11:A32:228:MET:HE1   | 1.57                     | 0.70              |
| 11:A32:437:LEU:HD11  | 11:A32:454:LYS:HZ3   | 1.56                     | 0.70              |
| 18:B8:1161:LEU:HD11  | 18:B8:1403:ILE:CG2   | 2.22                     | 0.70              |
| 3:N8:221:ASN:OD1     | 3:N8:224:LEU:N       | 2.22                     | 0.70              |
| 2:M16:231:ARG:HG3    | 2:M16:299:GLY:C      | 2.17                     | 0.70              |
| 2:M16:399:THR:CG2    | 2:M16:480:ARG:NH2    | 2.41                     | 0.70              |
| 2:M16:544:LEU:CD1    | 2:M16:586:ALA:HB1    | 2.21                     | 0.70              |
| 5:P:47:ASN:H         | 5:P:471:SER:HG       | 1.38                     | 0.70              |
| 8:L8:175:ARG:HH11    | 12:A48:134:LYS:HD3   | 1.56                     | 0.70              |
| 9:K:1019:ARG:HG2     | 9:K:1059:ARG:NH1     | 2.07                     | 0.70              |
| 9:K8:614:PHE:O       | 9:K8:683:GLN:NE2     | 2.24                     | 0.70              |
| 10:C24:18:THR:HG23   | 10:C24:883:GLU:HG2   | 1.73                     | 0.70              |
| 10:C24:565:ARG:HH22  | 10:C24:569:PHE:HD2   | 1.28                     | 0.70              |
| 10:C24:1466:ARG:HH12 | 11:A40:127:SER:HB3   | 1.55                     | 0.70              |
| 11:A40:24:ALA:O      | 23:J16:705:TRP:NE1   | 2.23                     | 0.70              |
| 11:A40:707:LEU:HD11  | 11:A40:767:ARG:HH12  | 1.55                     | 0.70              |
| 11:A40:803:PRO:CB    | 24:D24:1401:LEU:CD1  | 2.34                     | 0.70              |
| 12:A:707:LEU:HD21    | 12:A:767:ARG:NH2     | 2.07                     | 0.70              |
| 12:A:787:ASP:OD1     | 12:A:788:PRO:HD2     | 1.91                     | 0.70              |
| 10:C:847:ARG:CZ      | 10:C:903:ASN:CG      | 2.65                     | 0.70              |
| 10:C8:168:ARG:HH11   | 10:C8:229:PRO:HA     | 1.57                     | 0.70              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C8:847:ARG:CZ     | 10:C8:903:ASN:CG     | 2.65                     | 0.70              |
| 11:A16:90:PHE:CD2    | 18:B:1788:ILE:HD13   | 2.25                     | 0.70              |
| 18:B:234:TRP:CD2     | 18:B:309:MET:HE3     | 2.26                     | 0.70              |
| 20:E:73:ASP:OD1      | 20:E:96:ARG:NH2      | 2.24                     | 0.70              |
| 21:H:338:MET:CE      | 23:J32:692:VAL:HG21  | 2.21                     | 0.70              |
| 21:H16:312:GLN:CD    | 21:H16:316:ILE:HD11  | 2.16                     | 0.70              |
| 24:D16:1112:ALA:HB2  | 24:D16:1160:LEU:HD13 | 1.71                     | 0.70              |
| 10:C32:758:GLN:HE21  | 10:C32:819:GLN:HG2   | 1.54                     | 0.70              |
| 10:C32:847:ARG:NE    | 10:C32:903:ASN:CG    | 2.49                     | 0.70              |
| 10:C32:848:CYS:CA    | 10:C32:906:ARG:HH22  | 1.97                     | 0.70              |
| 10:C32:1133:ILE:HG13 | 10:C32:1152:LYS:NZ   | 2.05                     | 0.70              |
| 12:A48:212:LYS:CE    | 12:A48:585:MET:HE3   | 2.14                     | 0.70              |
| 1:R:1063:ARG:HE      | 24:D:1432:THR:HG21   | 1.57                     | 0.70              |
| 5:P8:55:ARG:CZ       | 5:P8:64:ASP:HB2      | 2.22                     | 0.70              |
| 8:L16:1071:LEU:HD21  | 9:K16:1284:MET:HE1   | 1.73                     | 0.70              |
| 10:C16:280:SER:O     | 10:C16:282:LYS:N     | 2.24                     | 0.70              |
| 10:C:847:ARG:NE      | 10:C:903:ASN:CG      | 2.50                     | 0.70              |
| 10:C8:1290:HIS:HB2   | 10:C8:1334:MET:HE3   | 1.70                     | 0.70              |
| 11:A16:273:ARG:NH2   | 11:A16:480:ASP:OD1   | 2.24                     | 0.70              |
| 11:A16:787:ASP:OD1   | 11:A16:788:PRO:HD2   | 1.91                     | 0.70              |
| 18:B:842:ASN:OD1     | 18:B:899:LYS:CE      | 2.40                     | 0.70              |
| 18:B8:842:ASN:OD1    | 18:B8:899:LYS:CE     | 2.40                     | 0.70              |
| 18:B8:1563:PHE:CE1   | 18:B8:1567:ILE:HD11  | 2.26                     | 0.70              |
| 20:E:429:PRO:HG3     | 24:D:69:VAL:CA       | 2.18                     | 0.70              |
| 21:H:280:LEU:HD21    | 22:I:262:LEU:HG      | 1.74                     | 0.70              |
| 21:H24:291:VAL:CG1   | 23:J24:657:GLU:HG3   | 2.21                     | 0.70              |
| 22:I16:131:ARG:NE    | 23:J16:557:ARG:HH21  | 1.88                     | 0.70              |
| 23:J16:718:GLN:CD    | 23:J16:737:TRP:HZ3   | 1.83                     | 0.70              |
| 12:A48:273:ARG:NH2   | 12:A48:480:ASP:OD1   | 2.24                     | 0.70              |
| 1:R:1124:TRP:HZ2     | 4:T:669:PRO:HG3      | 1.52                     | 0.70              |
| 2:M:639:GLN:HE22     | 3:N:269:LEU:HD13     | 0.75                     | 0.70              |
| 2:M8:625:HIS:NE2     | 3:N8:225:PRO:CA      | 2.55                     | 0.70              |
| 3:N16:162:THR:HG22   | 3:N16:168:VAL:CG2    | 2.16                     | 0.70              |
| 5:P:109:ILE:CD1      | 14:W:18:PRO:HG2      | 2.09                     | 0.70              |
| 7:Q8:125:TYR:HB3     | 7:Q8:168:LEU:HG      | 1.73                     | 0.70              |
| 7:Q8:200:PHE:CE2     | 7:Q8:228:ALA:HA      | 2.27                     | 0.70              |
| 8:L8:598:LEU:CD2     | 8:L8:627:ARG:NH1     | 2.55                     | 0.70              |
| 8:L8:608:PHE:CD2     | 8:L8:635:MET:SD      | 2.85                     | 0.70              |
| 9:K8:806:LEU:HD11    | 9:K8:839:LEU:HD11    | 1.73                     | 0.70              |
| 10:C16:470:HIS:HD2   | 10:C16:508:ILE:HD11  | 1.57                     | 0.70              |
| 11:A24:707:LEU:HD11  | 11:A24:767:ARG:HH12  | 1.55                     | 0.70              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A40:707:LEU:HD21 | 11:A40:767:ARG:NH2  | 2.07                     | 0.70              |
| 12:A:642:GLY:HA3    | 12:A:685:ARG:HH22   | 1.53                     | 0.70              |
| 10:C:35:ASN:OD1     | 24:D:1148:LEU:HD11  | 1.87                     | 0.70              |
| 10:C:922:ALA:HB1    | 10:C:923:PRO:HD2    | 1.74                     | 0.70              |
| 10:C:1770:LEU:O     | 10:C:1836:LYS:CE    | 2.38                     | 0.70              |
| 11:A16:70:GLU:O     | 21:H:351:ARG:NH1    | 2.24                     | 0.70              |
| 11:A32:52:LEU:CD2   | 11:A32:55:GLU:OE2   | 2.37                     | 0.70              |
| 18:B:729:LEU:HD13   | 18:B:1196:MET:SD    | 2.32                     | 0.70              |
| 21:H:312:GLN:CD     | 21:H:316:ILE:HD11   | 2.16                     | 0.70              |
| 22:I8:203:GLN:NE2   | 22:I8:209:TRP:HE1   | 1.89                     | 0.70              |
| 12:A48:787:ASP:OD1  | 12:A48:788:PRO:HD2  | 1.91                     | 0.70              |
| 2:M:202:LYS:NZ      | 2:M:208:SER:N       | 2.39                     | 0.70              |
| 2:M16:624:ASP:O     | 3:N16:165:GLY:CA    | 2.39                     | 0.70              |
| 2:M16:625:HIS:CD2   | 3:N16:225:PRO:HA    | 2.27                     | 0.70              |
| 2:M16:639:GLN:HE22  | 3:N16:269:LEU:HD13  | 0.75                     | 0.70              |
| 3:N16:4:GLN:NE2     | 3:N16:44:GLY:C      | 2.39                     | 0.70              |
| 5:P:600:PHE:HD2     | 5:P:638:SER:OG      | 1.68                     | 0.70              |
| 6:O8:105:ASN:ND2    | 6:O8:134:ARG:HH22   | 1.89                     | 0.70              |
| 5:P16:159:ILE:HD11  | 5:P16:214:LEU:CB    | 2.22                     | 0.70              |
| 7:Q16:125:TYR:HB3   | 7:Q16:168:LEU:HG    | 1.73                     | 0.70              |
| 9:K:783:ARG:HB3     | 9:K:785:ASP:OD1     | 1.91                     | 0.70              |
| 9:K8:831:SER:O      | 9:K8:882:SER:HB2    | 1.92                     | 0.70              |
| 11:A24:694:GLU:OE1  | 24:D8:1398:ARG:HA   | 1.91                     | 0.70              |
| 11:A24:707:LEU:HD21 | 11:A24:767:ARG:NH2  | 2.07                     | 0.70              |
| 10:C24:572:ILE:HG12 | 10:C24:606:MET:HE1  | 1.73                     | 0.70              |
| 10:C24:586:PRO:HD2  | 10:C24:650:ARG:HH11 | 1.54                     | 0.70              |
| 11:A40:390:ALA:HB1  | 24:D32:1099:ARG:CB  | 2.22                     | 0.70              |
| 14:W:584:CYS:SG     | 15:J:573:LYS:CG     | 2.79                     | 0.70              |
| 10:C:983:SER:HB3    | 10:C:1040:HIS:CD2   | 2.26                     | 0.70              |
| 10:C8:572:ILE:HG12  | 10:C8:606:MET:HE1   | 1.73                     | 0.70              |
| 11:A16:437:LEU:HD11 | 11:A16:454:LYS:HZ3  | 1.55                     | 0.70              |
| 11:A16:468:VAL:C    | 11:A16:470:LEU:H    | 2.00                     | 0.70              |
| 18:B:496:LEU:HD21   | 18:B:540:ILE:CD1    | 2.22                     | 0.70              |
| 21:H24:280:LEU:HD21 | 22:I24:262:LEU:HG   | 1.74                     | 0.70              |
| 21:H24:312:GLN:CD   | 21:H24:316:ILE:HD11 | 2.16                     | 0.70              |
| 2:M:628:LEU:HD12    | 3:N:223:GLY:CA      | 2.19                     | 0.70              |
| 2:M:672:TYR:CG      | 2:M:680:LYS:HD3     | 2.26                     | 0.70              |
| 4:T:672:GLN:CD      | 5:P:702:LEU:HD21    | 2.16                     | 0.70              |
| 5:P8:578:LEU:HD13   | 5:P8:608:LYS:HZ3    | 1.55                     | 0.70              |
| 7:Q16:200:PHE:CE2   | 7:Q16:228:ALA:HA    | 2.27                     | 0.70              |
| 8:L:621:SER:HB3     | 8:L:657:TYR:CD1     | 2.26                     | 0.70              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:L:1096:GLU:HG2    | 9:K:998:GLN:HE21    | 1.56                     | 0.70              |
| 9:K:1019:ARG:CD     | 9:K:1059:ARG:CD     | 2.69                     | 0.70              |
| 9:K:1048:GLN:OE1    | 9:K:1128:ARG:NE     | 2.25                     | 0.70              |
| 9:K8:1064:PRO:O     | 9:K8:1066:ASP:N     | 2.25                     | 0.70              |
| 10:C16:18:THR:HG23  | 10:C16:883:GLU:HG2  | 1.73                     | 0.70              |
| 10:C16:572:ILE:HG12 | 10:C16:606:MET:HE1  | 1.73                     | 0.70              |
| 11:A24:51:THR:HG23  | 22:I8:317:HIS:HB2   | 1.74                     | 0.70              |
| 10:C24:390:HIS:HB3  | 10:C24:452:LEU:HD23 | 1.74                     | 0.70              |
| 10:C24:698:PHE:CE2  | 10:C24:749:LEU:HD11 | 2.26                     | 0.70              |
| 10:C24:761:VAL:HG22 | 10:C24:826:TYR:CD1  | 2.26                     | 0.70              |
| 10:C:1716:LYS:HG3   | 10:C:1721:GLN:NE2   | 2.07                     | 0.70              |
| 11:A32:555:HIS:C    | 11:A32:557:LEU:N    | 2.50                     | 0.70              |
| 18:B:618:VAL:HG11   | 18:B:621:VAL:HG23   | 1.72                     | 0.70              |
| 18:B8:234:TRP:CE3   | 18:B8:309:MET:HE3   | 2.27                     | 0.70              |
| 18:B8:618:VAL:HG11  | 18:B8:621:VAL:CG2   | 2.22                     | 0.70              |
| 21:H16:287:ILE:HG23 | 22:I16:273:LEU:HD11 | 1.73                     | 0.70              |
| 10:C32:470:HIS:HD2  | 10:C32:508:ILE:HD11 | 1.57                     | 0.70              |
| 10:C32:619:LEU:HB3  | 10:C32:620:PRO:CD   | 2.19                     | 0.70              |
| 3:N8:4:GLN:NE2      | 3:N8:44:GLY:C       | 2.39                     | 0.70              |
| 3:N8:26:ILE:CD1     | 3:N8:40:VAL:HG21    | 2.21                     | 0.70              |
| 5:P16:55:ARG:CZ     | 5:P16:64:ASP:HB2    | 2.22                     | 0.70              |
| 10:C16:922:ALA:HB1  | 10:C16:923:PRO:HD2  | 1.74                     | 0.70              |
| 10:C16:1599:ASP:OD2 | 10:C16:1604:VAL:HB  | 1.91                     | 0.70              |
| 10:C24:470:HIS:HD2  | 10:C24:508:ILE:HD11 | 1.57                     | 0.70              |
| 10:C24:1068:THR:O   | 10:C24:1069:TYR:C   | 2.25                     | 0.70              |
| 11:A40:212:LYS:CE   | 11:A40:585:MET:HE3  | 2.14                     | 0.70              |
| 11:A40:362:ARG:HG2  | 11:A40:366:ARG:CZ   | 2.21                     | 0.70              |
| 10:C8:280:SER:O     | 10:C8:282:LYS:N     | 2.23                     | 0.70              |
| 10:C8:1716:LYS:HG3  | 10:C8:1721:GLN:NE2  | 2.07                     | 0.70              |
| 11:A32:70:GLU:O     | 21:H24:351:ARG:NH1  | 2.24                     | 0.70              |
| 11:A32:312:LEU:HD11 | 11:A32:364:ILE:HD11 | 1.71                     | 0.70              |
| 11:A32:707:LEU:HD21 | 11:A32:767:ARG:NH2  | 2.07                     | 0.70              |
| 18:B:421:ASP:CG     | 18:B:468:ARG:HH22   | 1.99                     | 0.70              |
| 18:B:989:ILE:O      | 18:B:991:ASP:N      | 2.25                     | 0.70              |
| 18:B:1110:LEU:HD23  | 21:H:326:GLY:CA     | 2.03                     | 0.70              |
| 18:B8:235:ARG:HH11  | 18:B8:308:GLU:HB3   | 1.56                     | 0.70              |
| 18:B8:1045:LYS:HZ1  | 18:B8:1100:LEU:HD21 | 1.57                     | 0.70              |
| 19:4:100:ILE:HD11   | 19:4:274:PHE:CE1    | 2.25                     | 0.70              |
| 22:I:210:LYS:C      | 22:I8:139:GLN:HE22  | 1.97                     | 0.70              |
| 21:H8:247:GLU:OE1   | 22:I8:184:VAL:HG11  | 1.92                     | 0.70              |
| 24:D16:1099:ARG:HG2 | 24:D16:1099:ARG:O   | 1.91                     | 0.70              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:453:LEU:HB2   | 10:C32:486:LEU:CD2   | 2.22                     | 0.70              |
| 10:C32:1271:PHE:CZ   | 10:C32:1284:ASP:CB   | 2.73                     | 0.70              |
| 12:A48:707:LEU:HD11  | 12:A48:767:ARG:HH12  | 1.55                     | 0.70              |
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:CG1    | 2.40                     | 0.69              |
| 2:M:625:HIS:NE2      | 3:N:225:PRO:CA       | 2.55                     | 0.69              |
| 1:R8:768:LEU:HG      | 24:D40:1362:VAL:C    | 2.17                     | 0.69              |
| 2:M16:672:TYR:HB2    | 2:M16:680:LYS:HD2    | 1.56                     | 0.69              |
| 5:P:16:PHE:HD1       | 6:O:311:LEU:CD1      | 2.03                     | 0.69              |
| 7:Q:200:PHE:CE2      | 7:Q:228:ALA:HA       | 2.27                     | 0.69              |
| 7:Q8:124:PHE:HD1     | 7:Q8:125:TYR:CD2     | 2.03                     | 0.69              |
| 8:L8:608:PHE:CD1     | 8:L8:635:MET:HG2     | 2.26                     | 0.69              |
| 10:C16:847:ARG:CZ    | 10:C16:903:ASN:CG    | 2.65                     | 0.69              |
| 11:A24:273:ARG:NH2   | 11:A24:480:ASP:OD1   | 2.24                     | 0.69              |
| 10:C24:663:ILE:CG2   | 10:C24:667:ILE:HD11  | 2.22                     | 0.69              |
| 12:A:555:HIS:C       | 12:A:557:LEU:N       | 2.50                     | 0.69              |
| 13:V:847:ASN:HD22    | 14:W:723:TYR:HE1     | 1.38                     | 0.69              |
| 10:C:619:LEU:HB3     | 10:C:620:PRO:CD      | 2.19                     | 0.69              |
| 10:C8:795:ASP:OD2    | 10:C8:850:ARG:NH1    | 2.25                     | 0.69              |
| 11:A32:273:ARG:NH2   | 11:A32:480:ASP:OD1   | 2.24                     | 0.69              |
| 11:A32:732:TYR:OH    | 11:A32:743:ARG:HG2   | 1.92                     | 0.69              |
| 18:B:90:ILE:HD12     | 18:B:105:VAL:HG22    | 1.72                     | 0.69              |
| 18:B8:90:ILE:HD12    | 18:B8:105:VAL:HG22   | 1.72                     | 0.69              |
| 18:B8:428:GLN:HG3    | 18:B8:584:ARG:CZ     | 2.11                     | 0.69              |
| 19:48:183:ARG:HH12   | 19:48:245:GLY:N      | 1.88                     | 0.69              |
| 2:M8:627:TYR:HE2     | 3:N8:162:THR:HB      | 1.56                     | 0.69              |
| 5:P:402:LEU:CD2      | 5:P:433:LEU:HD13     | 2.19                     | 0.69              |
| 9:K:916:LYS:HG3      | 9:K:919:MET:CE       | 2.21                     | 0.69              |
| 11:A24:803:PRO:CB    | 24:D8:1401:LEU:CD1   | 2.44                     | 0.69              |
| 10:C24:1724:VAL:HG22 | 10:C24:1736:ILE:HD12 | 1.72                     | 0.69              |
| 11:A40:56:ALA:C      | 11:A40:58:SER:N      | 2.49                     | 0.69              |
| 10:C:18:THR:HG21     | 10:C:883:GLU:HG2     | 1.73                     | 0.69              |
| 10:C:572:ILE:HG12    | 10:C:606:MET:HE1     | 1.73                     | 0.69              |
| 10:C:1251:PHE:HZ     | 10:C:1319:ARG:CZ     | 1.99                     | 0.69              |
| 10:C8:572:ILE:HD13   | 10:C8:606:MET:CE     | 2.18                     | 0.69              |
| 10:C8:1166:SER:O     | 10:C8:1168:PRO:N     | 2.24                     | 0.69              |
| 18:B:712:PRO:HB3     | 18:B:759:MET:HE2     | 1.75                     | 0.69              |
| 18:B:1793:ILE:O      | 18:B:1794:SER:C      | 2.30                     | 0.69              |
| 18:B8:583:ARG:NH2    | 18:B8:711:CYS:HB2    | 2.06                     | 0.69              |
| 18:B8:856:LEU:CD1    | 18:B8:907:SER:HB2    | 2.22                     | 0.69              |
| 18:B8:1215:PHE:HE1   | 18:B8:1234:MET:SD    | 2.13                     | 0.69              |
| 21:H8:312:GLN:CD     | 21:H8:316:ILE:HD11   | 2.16                     | 0.69              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D32:764:GLU:OE1   | 24:D40:620:GLN:CD    | 2.35                     | 0.69              |
| 24:D40:865:VAL:HG21  | 24:D40:928:THR:HG21  | 1.74                     | 0.69              |
| 10:C32:1318:ARG:HH21 | 10:C32:1396:SER:HG   | 1.37                     | 0.69              |
| 12:A48:468:VAL:C     | 12:A48:470:LEU:H     | 1.99                     | 0.69              |
| 12:A48:555:HIS:C     | 12:A48:557:LEU:N     | 2.50                     | 0.69              |
| 1:R:979:GLN:HB2      | 24:D:1438:ALA:HB2    | 1.74                     | 0.69              |
| 2:M:651:ARG:HG3      | 2:M:664:MET:HE1      | 1.73                     | 0.69              |
| 1:R8:1115:TYR:HB2    | 1:R8:1131:MET:HE3    | 1.73                     | 0.69              |
| 2:M16:451:PHE:O      | 8:L16:295:HIS:CD2    | 2.46                     | 0.69              |
| 5:P:401:ARG:CD       | 5:P:414:VAL:CB       | 2.69                     | 0.69              |
| 5:P:401:ARG:HG2      | 5:P:414:VAL:CG1      | 2.16                     | 0.69              |
| 5:P:401:ARG:NH2      | 5:P:404:ILE:HG22     | 2.07                     | 0.69              |
| 7:Q:149:VAL:HG23     | 7:Q:187:TRP:CE2      | 2.26                     | 0.69              |
| 5:P16:55:ARG:HH12    | 5:P16:64:ASP:CB      | 1.97                     | 0.69              |
| 10:C16:663:ILE:CG2   | 10:C16:667:ILE:HD11  | 2.22                     | 0.69              |
| 10:C16:1663:SER:C    | 10:C24:1568:ARG:NH2  | 2.51                     | 0.69              |
| 12:A:144:LYS:CE      | 10:C:1821:VAL:HG11   | 2.22                     | 0.69              |
| 10:C:663:ILE:CG2     | 10:C:667:ILE:HD11    | 2.22                     | 0.69              |
| 10:C8:1251:PHE:HZ    | 10:C8:1319:ARG:CZ    | 1.99                     | 0.69              |
| 10:C8:1766:ILE:HD13  | 10:C8:1800:LEU:HD21  | 1.74                     | 0.69              |
| 10:C8:1821:VAL:HG11  | 16:A8:144:LYS:CE     | 2.22                     | 0.69              |
| 11:A16:121:GLN:HE22  | 18:B:1559:ALA:HB1    | 1.57                     | 0.69              |
| 17:F8:73:GLY:O       | 17:F8:75:ALA:N       | 2.25                     | 0.69              |
| 17:F:73:GLY:O        | 17:F:75:ALA:N        | 2.25                     | 0.69              |
| 11:A32:706:SER:HB3   | 24:D32:1398:ARG:HG2  | 1.73                     | 0.69              |
| 11:A32:707:LEU:HD11  | 11:A32:767:ARG:HH12  | 1.55                     | 0.69              |
| 18:B:618:VAL:HG11    | 18:B:621:VAL:CG2     | 2.22                     | 0.69              |
| 18:B:1222:TYR:OH     | 18:B:1240:ASP:OD2    | 2.07                     | 0.69              |
| 18:B8:496:LEU:HD21   | 18:B8:540:ILE:CD1    | 2.22                     | 0.69              |
| 18:B8:618:VAL:HG11   | 18:B8:621:VAL:HG23   | 1.72                     | 0.69              |
| 18:B8:729:LEU:HD13   | 18:B8:1196:MET:SD    | 2.32                     | 0.69              |
| 18:B8:989:ILE:O      | 18:B8:991:ASP:N      | 2.25                     | 0.69              |
| 22:I24:131:ARG:HG3   | 23:J24:557:ARG:HH22  | 1.46                     | 0.69              |
| 10:C32:1766:ILE:HD13 | 10:C32:1800:LEU:HD21 | 1.74                     | 0.69              |
| 12:A48:732:TYR:OH    | 12:A48:743:ARG:HG2   | 1.92                     | 0.69              |
| 2:M8:221:LYS:HD3     | 3:N8:301:GLU:OE2     | 1.93                     | 0.69              |
| 2:M16:221:LYS:HD3    | 3:N16:301:GLU:OE2    | 1.93                     | 0.69              |
| 6:O16:105:ASN:ND2    | 6:O16:134:ARG:HH22   | 1.89                     | 0.69              |
| 9:K:806:LEU:HD11     | 9:K:839:LEU:HD11     | 1.73                     | 0.69              |
| 9:K:1048:GLN:NE2     | 9:K:1128:ARG:HG2     | 2.07                     | 0.69              |
| 9:K:1056:VAL:HG21    | 9:K:1059:ARG:HH21    | 1.56                     | 0.69              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A24:555:HIS:C     | 11:A24:557:LEU:N     | 2.50                     | 0.69              |
| 10:C24:847:ARG:CZ    | 10:C24:903:ASN:CG    | 2.65                     | 0.69              |
| 10:C24:1271:PHE:CZ   | 10:C24:1284:ASP:OD1  | 2.29                     | 0.69              |
| 11:A40:468:VAL:C     | 11:A40:470:LEU:H     | 2.00                     | 0.69              |
| 14:W:554:LYS:CD      | 14:W:597:ARG:NH2     | 2.54                     | 0.69              |
| 10:C:153:ALA:HB3     | 24:D:1403:LEU:CG     | 1.97                     | 0.69              |
| 10:C:453:LEU:CD1     | 10:C:486:LEU:CD2     | 2.70                     | 0.69              |
| 10:C8:453:LEU:CD1    | 10:C8:486:LEU:CD2    | 2.70                     | 0.69              |
| 11:A16:259:ILE:HG22  | 11:A16:276:LEU:HD22  | 1.75                     | 0.69              |
| 11:A16:555:HIS:C     | 11:A16:557:LEU:N     | 2.50                     | 0.69              |
| 11:A16:732:TYR:OH    | 11:A16:743:ARG:HG2   | 1.92                     | 0.69              |
| 18:B:282:GLU:HG3     | 18:B:444:VAL:CG2     | 2.22                     | 0.69              |
| 18:B:856:LEU:CD1     | 18:B:907:SER:HB2     | 2.22                     | 0.69              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:CG2    | 2.22                     | 0.69              |
| 18:B:1587:ARG:HG3    | 18:B:1650:TYR:CE2    | 2.28                     | 0.69              |
| 18:B8:282:GLU:HG3    | 18:B8:444:VAL:CG2    | 2.22                     | 0.69              |
| 19:48:100:ILE:HD11   | 19:48:274:PHE:CE1    | 2.25                     | 0.69              |
| 21:H:247:GLU:OE1     | 22:I:184:VAL:HG11    | 1.92                     | 0.69              |
| 1:R16:1225:PHE:HE1   | 1:R16:1247:PRO:HB3   | 1.58                     | 0.69              |
| 5:P:55:ARG:CZ        | 5:P:64:ASP:HB2       | 2.22                     | 0.69              |
| 7:Q:125:TYR:HB3      | 7:Q:168:LEU:HG       | 1.73                     | 0.69              |
| 9:K:725:SER:OG       | 9:K:726:GLU:N        | 2.25                     | 0.69              |
| 9:K8:725:SER:OG      | 9:K8:726:GLU:N       | 2.25                     | 0.69              |
| 9:K8:1048:GLN:OE1    | 9:K8:1128:ARG:NE     | 2.25                     | 0.69              |
| 10:C16:848:CYS:CA    | 10:C16:906:ARG:HH22  | 1.97                     | 0.69              |
| 10:C16:1352:GLN:CD   | 10:C16:1357:LEU:HD12 | 2.18                     | 0.69              |
| 11:A24:468:VAL:C     | 11:A24:470:LEU:H     | 2.00                     | 0.69              |
| 11:A24:468:VAL:HG11  | 24:D16:1100:GLN:CB   | 2.23                     | 0.69              |
| 10:C24:280:SER:O     | 10:C24:282:LYS:N     | 2.24                     | 0.69              |
| 10:C24:1766:ILE:HD13 | 10:C24:1800:LEU:HD21 | 1.74                     | 0.69              |
| 10:C24:1821:VAL:HG11 | 11:A40:144:LYS:CE    | 2.22                     | 0.69              |
| 11:A40:555:HIS:C     | 11:A40:557:LEU:N     | 2.50                     | 0.69              |
| 13:V:895:LEU:HD21    | 14:W:774:MET:HE1     | 1.73                     | 0.69              |
| 14:W:746:THR:HG22    | 15:J:675:ASN:ND2     | 2.06                     | 0.69              |
| 10:C:1352:GLN:CD     | 10:C:1357:LEU:HD12   | 2.18                     | 0.69              |
| 18:B:284:LEU:HD11    | 18:B:334:PHE:CE2     | 2.28                     | 0.69              |
| 18:B:1848:VAL:HG12   | 18:B:1850:TYR:CE1    | 2.27                     | 0.69              |
| 18:B8:7:VAL:HG11     | 18:B8:99:ILE:HD12    | 1.75                     | 0.69              |
| 18:B8:421:ASP:CG     | 18:B8:468:ARG:HH22   | 1.99                     | 0.69              |
| 18:B8:536:ILE:CG2    | 18:B8:545:VAL:CG1    | 2.58                     | 0.69              |
| 18:B8:1119:LYS:O     | 18:B8:1120:THR:O     | 2.10                     | 0.69              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1156:GLN:C     | 18:B8:1382:LYS:NZ    | 2.50                     | 0.69              |
| 20:E8:33:PHE:HD1     | 20:E8:37:LEU:HD12    | 1.58                     | 0.69              |
| 21:H16:280:LEU:HD21  | 22:I16:262:LEU:HG    | 1.74                     | 0.69              |
| 24:D:405:GLN:HA      | 24:D16:10:ARG:HH11   | 1.57                     | 0.69              |
| 10:C32:1033:GLY:C    | 10:C32:1218:ARG:HH22 | 2.01                     | 0.69              |
| 10:C32:1821:VAL:HG11 | 12:A48:144:LYS:CE    | 2.22                     | 0.69              |
| 2:M:328:THR:HG21     | 2:M:350:SER:OG       | 1.93                     | 0.69              |
| 1:R8:1225:PHE:HE1    | 1:R8:1247:PRO:HB3    | 1.58                     | 0.69              |
| 3:N8:162:THR:HG22    | 3:N8:168:VAL:CG2     | 2.16                     | 0.69              |
| 2:M16:625:HIS:NE2    | 3:N16:225:PRO:CA     | 2.55                     | 0.69              |
| 9:K8:1048:GLN:NE2    | 9:K8:1128:ARG:HG2    | 2.07                     | 0.69              |
| 10:C16:228:ARG:HH22  | 10:C16:277:SER:HB3   | 1.57                     | 0.69              |
| 11:A24:732:TYR:OH    | 11:A24:743:ARG:HG2   | 1.92                     | 0.69              |
| 10:C24:1352:GLN:CD   | 10:C24:1357:LEU:HD12 | 2.18                     | 0.69              |
| 12:A:437:LEU:HD11    | 12:A:454:LYS:CE      | 2.23                     | 0.69              |
| 10:C:668:ALA:N       | 10:C:700:MET:HE1     | 2.08                     | 0.69              |
| 10:C:1286:MET:HE3    | 10:C:1344:VAL:HG11   | 1.73                     | 0.69              |
| 10:C:1777:SER:O      | 10:C:1778:ASN:C      | 2.27                     | 0.69              |
| 10:C8:1352:GLN:CD    | 10:C8:1357:LEU:HD12  | 2.18                     | 0.69              |
| 11:A32:764:LYS:HE2   | 19:48:36:LYS:NZ      | 2.07                     | 0.69              |
| 18:B:234:TRP:CE3     | 18:B:309:MET:HE3     | 2.27                     | 0.69              |
| 18:B:235:ARG:HH11    | 18:B:308:GLU:HB3     | 1.56                     | 0.69              |
| 18:B:1119:LYS:O      | 18:B:1120:THR:O      | 2.10                     | 0.69              |
| 18:B8:495:THR:HG23   | 18:B8:549:TRP:HE1    | 1.58                     | 0.69              |
| 20:E8:358:GLY:CA     | 20:E8:454:MET:SD     | 2.77                     | 0.69              |
| 22:I:131:ARG:HE      | 23:J32:557:ARG:NH2   | 1.91                     | 0.69              |
| 22:I24:131:ARG:HE    | 23:J24:557:ARG:NH2   | 1.91                     | 0.69              |
| 21:H16:291:VAL:CG1   | 23:J16:657:GLU:HG3   | 2.21                     | 0.69              |
| 24:D:1431:MET:HB3    | 24:D:1435:ARG:HH12   | 1.58                     | 0.69              |
| 12:A48:707:LEU:HD21  | 12:A48:767:ARG:NH2   | 2.07                     | 0.69              |
| 2:M:221:LYS:HD3      | 3:N:301:GLU:OE2      | 1.93                     | 0.69              |
| 2:M8:328:THR:HG21    | 2:M8:350:SER:CB      | 2.21                     | 0.69              |
| 2:M8:639:GLN:HE22    | 3:N8:269:LEU:HD13    | 0.75                     | 0.69              |
| 1:R16:1115:TYR:HB2   | 1:R16:1131:MET:HE3   | 1.73                     | 0.69              |
| 5:P8:159:ILE:HD11    | 5:P8:214:LEU:CB      | 2.22                     | 0.69              |
| 7:Q16:297:VAL:HG13   | 7:Q16:301:ARG:CD     | 2.23                     | 0.69              |
| 9:K:703:LEU:HD13     | 9:K:805:ILE:HD11     | 1.74                     | 0.69              |
| 9:K8:994:TYR:HD2     | 9:K8:1023:LEU:HD11   | 1.55                     | 0.69              |
| 10:C16:300:VAL:CG1   | 10:C16:317:ARG:HG3   | 2.23                     | 0.69              |
| 10:C16:453:LEU:HB2   | 10:C16:486:LEU:CD2   | 2.22                     | 0.69              |
| 10:C16:1278:ASP:OD2  | 21:H:283:LYS:HA      | 1.92                     | 0.69              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1286:MET:HE3  | 10:C16:1344:VAL:HG11 | 1.73                     | 0.69              |
| 10:C16:1821:VAL:HG11 | 11:A24:144:LYS:CE    | 2.22                     | 0.69              |
| 10:C24:847:ARG:NH2   | 10:C24:911:ILE:N     | 2.41                     | 0.69              |
| 10:C24:1814:LYS:HE2  | 23:J24:738:MET:HE2   | 1.74                     | 0.69              |
| 11:A40:36:ASN:ND2    | 22:I16:293:LYS:HZ1   | 1.88                     | 0.69              |
| 11:A40:51:THR:HG23   | 22:I16:317:HIS:HB2   | 1.74                     | 0.69              |
| 11:A40:273:ARG:NH2   | 11:A40:480:ASP:OD1   | 2.24                     | 0.69              |
| 11:A40:732:TYR:OH    | 11:A40:743:ARG:HG2   | 1.92                     | 0.69              |
| 10:C:300:VAL:CG1     | 10:C:317:ARG:HG3     | 2.23                     | 0.69              |
| 10:C8:470:HIS:HD2    | 10:C8:508:ILE:HD11   | 1.57                     | 0.69              |
| 10:C8:1286:MET:HE3   | 10:C8:1344:VAL:HG11  | 1.73                     | 0.69              |
| 11:A32:259:ILE:HG22  | 11:A32:276:LEU:HD22  | 1.75                     | 0.69              |
| 18:B:7:VAL:HG11      | 18:B:99:ILE:HD12     | 1.75                     | 0.69              |
| 20:E:25:PRO:HG3      | 20:E:237:ILE:HD11    | 1.72                     | 0.69              |
| 21:H24:247:GLU:OE1   | 22:I24:184:VAL:HG11  | 1.92                     | 0.69              |
| 2:M:672:TYR:CE1      | 2:M:680:LYS:NZ       | 2.59                     | 0.69              |
| 2:M8:627:TYR:H       | 2:M8:627:TYR:HD1     | 1.37                     | 0.69              |
| 5:P:207:HIS:HB3      | 5:P:208:PRO:HD2      | 1.74                     | 0.69              |
| 5:P:402:LEU:HD11     | 5:P:433:LEU:HB3      | 1.71                     | 0.69              |
| 8:L8:1096:GLU:CD     | 9:K8:996:MET:O       | 2.35                     | 0.69              |
| 9:K:869:GLU:OE1      | 9:K:944:ASN:CB       | 2.39                     | 0.69              |
| 9:K:923:ILE:CG2      | 9:K:929:ARG:NE       | 2.53                     | 0.69              |
| 9:K:1110:GLN:O       | 9:K:1114:THR:OG1     | 2.09                     | 0.69              |
| 9:K8:1025:TRP:CZ2    | 9:K8:1026:LEU:HD12   | 2.28                     | 0.69              |
| 10:C16:847:ARG:NH2   | 10:C16:911:ILE:N     | 2.41                     | 0.69              |
| 10:C16:1163:LEU:HD23 | 10:C16:1166:SER:HG   | 1.56                     | 0.69              |
| 10:C16:1547:LYS:CE   | 24:D8:1405:GLY:N     | 2.55                     | 0.69              |
| 10:C16:1716:LYS:HG3  | 10:C16:1721:GLN:NE2  | 2.07                     | 0.69              |
| 10:C24:593:ARG:HH12  | 10:C24:655:SER:HG    | 1.41                     | 0.69              |
| 10:C24:922:ALA:HB1   | 10:C24:923:PRO:HD2   | 1.74                     | 0.69              |
| 11:A40:225:ARG:HH11  | 11:A40:228:MET:HE1   | 1.57                     | 0.69              |
| 12:A:732:TYR:OH      | 12:A:743:ARG:HG2     | 1.92                     | 0.69              |
| 13:V:925:ILE:HD11    | 14:W:801:ALA:CB      | 2.23                     | 0.69              |
| 14:W:638:VAL:HG21    | 15:J:561:PHE:CZ      | 2.28                     | 0.69              |
| 10:C:847:ARG:NH2     | 10:C:911:ILE:N       | 2.41                     | 0.69              |
| 10:C8:1777:SER:O     | 10:C8:1778:ASN:C     | 2.26                     | 0.69              |
| 11:A16:713:ASP:OD2   | 11:A16:717:ARG:NE    | 2.24                     | 0.69              |
| 18:B:729:LEU:HB2     | 18:B:1196:MET:HE3    | 1.73                     | 0.69              |
| 18:B8:284:LEU:HD11   | 18:B8:334:PHE:CE2    | 2.28                     | 0.69              |
| 18:B8:985:ASP:O      | 18:B8:986:ALA:C      | 2.24                     | 0.69              |
| 18:B8:1110:LEU:HD21  | 21:H24:326:GLY:HA2   | 1.74                     | 0.69              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1529:GLU:OE2   | 24:D32:1415:LEU:HD21 | 1.92                     | 0.69              |
| 18:B8:1848:VAL:HG12  | 18:B8:1850:TYR:CE1   | 2.27                     | 0.69              |
| 21:H8:287:ILE:HG23   | 22:I8:273:LEU:HD11   | 1.73                     | 0.69              |
| 21:H16:247:GLU:OE1   | 22:I16:184:VAL:HG11  | 1.92                     | 0.69              |
| 21:H16:366:MET:SD    | 22:I16:332:MET:HE3   | 2.32                     | 0.69              |
| 22:I16:131:ARG:CG    | 23:J16:557:ARG:HH21  | 1.80                     | 0.69              |
| 10:C32:18:THR:HG23   | 10:C32:883:GLU:HG2   | 1.73                     | 0.69              |
| 10:C32:300:VAL:CG1   | 10:C32:317:ARG:HG3   | 2.23                     | 0.69              |
| 10:C32:572:ILE:HD13  | 10:C32:606:MET:CE    | 2.18                     | 0.69              |
| 10:C32:922:ALA:HB1   | 10:C32:923:PRO:HD2   | 1.74                     | 0.69              |
| 10:C32:1708:ARG:HG3  | 10:C32:1730:ILE:HD12 | 1.72                     | 0.69              |
| 12:A48:225:ARG:HH11  | 12:A48:228:MET:HE1   | 1.57                     | 0.69              |
| 1:R8:1115:TYR:HB2    | 1:R8:1131:MET:CE     | 2.23                     | 0.69              |
| 2:M8:540:TYR:CD1     | 2:M8:555:LEU:HD23    | 2.28                     | 0.69              |
| 7:Q:295:SER:HB2      | 7:Q:297:VAL:HG23     | 1.73                     | 0.69              |
| 5:P8:313:TRP:CZ2     | 5:P8:345:MET:HE3     | 2.13                     | 0.69              |
| 9:K:831:SER:O        | 9:K:882:SER:HB2      | 1.92                     | 0.69              |
| 9:K:1064:PRO:O       | 9:K:1066:ASP:N       | 2.25                     | 0.69              |
| 10:C16:717:GLU:HG2   | 23:J8:656:ARG:HE     | 1.56                     | 0.69              |
| 10:C16:1033:GLY:C    | 10:C16:1218:ARG:HH22 | 2.01                     | 0.69              |
| 10:C16:1766:ILE:HD13 | 10:C16:1800:LEU:HD21 | 1.74                     | 0.69              |
| 11:A40:440:LEU:HD12  | 11:A40:443:LEU:HD11  | 1.75                     | 0.69              |
| 10:C:1158:HIS:CE1    | 10:C:1164:VAL:HG11   | 2.28                     | 0.69              |
| 10:C:1285:VAL:HG21   | 10:C:1738:MET:HE3    | 1.61                     | 0.69              |
| 10:C8:668:ALA:N      | 10:C8:700:MET:HE1    | 2.07                     | 0.69              |
| 11:A16:706:SER:HB2   | 24:D16:1398:ARG:CG   | 2.22                     | 0.69              |
| 18:B:495:THR:HG23    | 18:B:549:TRP:HE1     | 1.58                     | 0.69              |
| 18:B:583:ARG:CZ      | 18:B:711:CYS:CB      | 2.67                     | 0.69              |
| 18:B:1156:GLN:C      | 18:B:1382:LYS:NZ     | 2.50                     | 0.69              |
| 18:B8:1349:LEU:HD22  | 18:B8:1367:ILE:HD11  | 1.75                     | 0.69              |
| 18:B8:1587:ARG:HG3   | 18:B8:1650:TYR:CE2   | 2.28                     | 0.69              |
| 20:E8:202:ASP:C      | 20:E8:204:SER:N      | 2.47                     | 0.69              |
| 10:C32:26:ARG:HH21   | 10:C32:151:LEU:HB2   | 1.58                     | 0.69              |
| 10:C32:847:ARG:NH2   | 10:C32:911:ILE:N     | 2.41                     | 0.69              |
| 1:R:1473:HIS:CD2     | 6:O:160:LEU:HD22     | 2.27                     | 0.69              |
| 2:M8:544:LEU:HD11    | 2:M8:586:ALA:O       | 1.92                     | 0.69              |
| 1:R16:1115:TYR:HB2   | 1:R16:1131:MET:CE    | 2.23                     | 0.69              |
| 2:M16:420:CYS:CB     | 8:L16:391:TRP:CZ3    | 2.75                     | 0.69              |
| 5:P8:98:PRO:HA       | 5:P8:133:TYR:OH      | 1.93                     | 0.69              |
| 5:P16:458:GLU:OE1    | 5:P16:462:ARG:NH2    | 2.26                     | 0.69              |
| 8:L16:1031:PRO:HA    | 8:L16:1068:PHE:HZ    | 1.57                     | 0.69              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 9:K:1025:TRP:CZ2     | 9:K:1026:LEU:HD12   | 2.28                     | 0.69              |
| 10:C24:407:LYS:NZ    | 10:C24:465:PHE:CE2  | 2.53                     | 0.69              |
| 10:C24:1166:SER:O    | 10:C24:1168:PRO:N   | 2.24                     | 0.69              |
| 10:C24:1280:VAL:HG22 | 10:C24:1731:HIS:ND1 | 2.08                     | 0.69              |
| 10:C:407:LYS:HG3     | 10:C:465:PHE:CZ     | 2.28                     | 0.69              |
| 10:C:470:HIS:HD2     | 10:C:508:ILE:HD11   | 1.57                     | 0.69              |
| 10:C:795:ASP:OD2     | 10:C:850:ARG:NH1    | 2.25                     | 0.69              |
| 10:C8:278:ARG:HH11   | 10:C8:287:SER:HB2   | 1.56                     | 0.69              |
| 11:A32:713:ASP:OD2   | 11:A32:717:ARG:NE   | 2.25                     | 0.69              |
| 17:F24:73:GLY:O      | 17:F24:75:ALA:N     | 2.25                     | 0.69              |
| 18:B:683:ASN:C       | 18:B:685:SER:H      | 2.01                     | 0.69              |
| 18:B:690:TRP:CH2     | 18:B:787:VAL:HG22   | 2.26                     | 0.69              |
| 18:B:1349:LEU:HD22   | 18:B:1367:ILE:HD11  | 1.75                     | 0.69              |
| 18:B:1719:SER:HB3    | 18:B:1720:PRO:HD3   | 1.74                     | 0.69              |
| 18:B8:583:ARG:CZ     | 18:B8:711:CYS:CB    | 2.67                     | 0.69              |
| 21:H:366:MET:SD      | 22:I:332:MET:HE3    | 2.32                     | 0.69              |
| 24:D:400:VAL:CB      | 24:D16:751:MET:HB2  | 2.22                     | 0.69              |
| 10:C32:572:ILE:HG12  | 10:C32:606:MET:HE1  | 1.73                     | 0.69              |
| 1:R8:1078:SER:CB     | 5:P8:713:LEU:HD21   | 2.24                     | 0.68              |
| 1:R8:1203:SER:O      | 1:R8:1205:ASP:N     | 2.26                     | 0.68              |
| 2:M8:625:HIS:CD2     | 3:N8:225:PRO:HA     | 2.27                     | 0.68              |
| 1:R16:1261:TYR:OH    | 1:R16:1291:LYS:NZ   | 2.26                     | 0.68              |
| 2:M16:328:THR:HG21   | 2:M16:350:SER:OG    | 1.93                     | 0.68              |
| 9:K8:955:TYR:CZ      | 9:K8:985:PHE:CA     | 2.76                     | 0.68              |
| 10:C16:26:ARG:HH21   | 10:C16:151:LEU:HB2  | 1.58                     | 0.68              |
| 10:C16:1661:LEU:O    | 10:C16:1662:ASP:C   | 2.29                     | 0.68              |
| 12:A:642:GLY:CA      | 12:A:685:ARG:NH1    | 2.40                     | 0.68              |
| 12:A:704:ILE:HG12    | 12:A:760:LEU:HD12   | 1.75                     | 0.68              |
| 14:W:517:GLU:CD      | 14:W:605:ASN:O      | 2.36                     | 0.68              |
| 18:B8:111:GLN:OE1    | 18:B8:134:GLN:NE2   | 2.25                     | 0.68              |
| 18:B8:671:MET:HE2    | 18:B8:736:ALA:HB2   | 1.67                     | 0.68              |
| 18:B8:1256:THR:HG23  | 24:D32:1238:GLU:CG  | 2.17                     | 0.68              |
| 19:48:100:ILE:CD1    | 19:48:274:PHE:CE1   | 2.76                     | 0.68              |
| 20:E8:430:ALA:O      | 20:E8:431:SER:C     | 2.28                     | 0.68              |
| 21:H8:366:MET:SD     | 22:I8:332:MET:HE3   | 2.32                     | 0.68              |
| 10:C32:586:PRO:HD2   | 10:C32:650:ARG:HH11 | 1.54                     | 0.68              |
| 12:A48:437:LEU:HD11  | 12:A48:454:LYS:CE   | 2.23                     | 0.68              |
| 2:M8:672:TYR:CD2     | 2:M8:680:LYS:HD3    | 2.25                     | 0.68              |
| 7:Q8:295:SER:HB2     | 7:Q8:297:VAL:HG23   | 1.73                     | 0.68              |
| 5:P16:16:PHE:CE2     | 5:P16:461:HIS:NE2   | 2.61                     | 0.68              |
| 8:L16:1069:LEU:HD21  | 9:K16:1086:VAL:HG21 | 1.75                     | 0.68              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:806:LEU:HD13     | 9:K:874:VAL:HG12     | 1.74                     | 0.68              |
| 9:K:1154:TRP:CE2     | 9:K:1219:VAL:HG11    | 2.25                     | 0.68              |
| 9:K8:1085:TYR:CZ     | 9:K8:1093:SER:HB2    | 2.14                     | 0.68              |
| 10:C16:1061:ASN:O    | 10:C16:1062:GLU:C    | 2.25                     | 0.68              |
| 10:C16:1665:THR:HG21 | 10:C24:1600:GLY:O    | 1.93                     | 0.68              |
| 10:C24:26:ARG:HH21   | 10:C24:151:LEU:HB2   | 1.58                     | 0.68              |
| 10:C24:1033:GLY:C    | 10:C24:1218:ARG:HH22 | 2.01                     | 0.68              |
| 10:C:452:LEU:HD11    | 10:C:453:LEU:CG      | 2.14                     | 0.68              |
| 10:C:1033:GLY:C      | 10:C:1218:ARG:HH22   | 2.01                     | 0.68              |
| 10:C8:300:VAL:CG1    | 10:C8:317:ARG:HG3    | 2.23                     | 0.68              |
| 10:C8:847:ARG:NH2    | 10:C8:911:ILE:N      | 2.41                     | 0.68              |
| 11:A16:51:THR:HG23   | 22:I:317:HIS:HB2     | 1.74                     | 0.68              |
| 11:A16:225:ARG:HH11  | 11:A16:228:MET:HE1   | 1.56                     | 0.68              |
| 11:A16:437:LEU:HD11  | 11:A16:454:LYS:CE    | 2.23                     | 0.68              |
| 11:A16:707:LEU:HD21  | 11:A16:767:ARG:NH2   | 2.07                     | 0.68              |
| 18:B:113:TYR:HE1     | 18:B:119:VAL:HG11    | 1.57                     | 0.68              |
| 18:B:660:ALA:HB3     | 18:B:661:PRO:HD3     | 1.76                     | 0.68              |
| 18:B8:686:LEU:HD11   | 18:B8:790:ASP:CG     | 2.17                     | 0.68              |
| 18:B8:1291:LEU:HD12  | 18:B8:1332:VAL:CG2   | 2.21                     | 0.68              |
| 20:E:341:TYR:O       | 20:E:342:GLN:C       | 2.27                     | 0.68              |
| 20:E:430:ALA:O       | 20:E:431:SER:C       | 2.28                     | 0.68              |
| 21:H24:366:MET:SD    | 22:I24:332:MET:HE3   | 2.32                     | 0.68              |
| 10:C32:278:ARG:HH11  | 10:C32:287:SER:HB2   | 1.56                     | 0.68              |
| 10:C32:1716:LYS:HG3  | 10:C32:1721:GLN:NE2  | 2.07                     | 0.68              |
| 1:R:1225:PHE:HE1     | 1:R:1247:PRO:HB3     | 1.58                     | 0.68              |
| 1:R:1331:GLY:O       | 10:C:1170:VAL:HG22   | 1.94                     | 0.68              |
| 1:R8:982:GLU:OE1     | 24:D40:1436:ARG:HG2  | 1.93                     | 0.68              |
| 2:M8:547:LYS:NZ      | 2:M8:554:PHE:CZ      | 2.60                     | 0.68              |
| 2:M8:819:GLN:OE1     | 2:M8:846:LEU:HD21    | 1.92                     | 0.68              |
| 1:R16:1379:GLN:NE2   | 1:R16:1416:TYR:HE1   | 1.92                     | 0.68              |
| 2:M16:351:ALA:HB1    | 8:L16:219:ILE:HG23   | 1.70                     | 0.68              |
| 5:P16:16:PHE:HD1     | 6:O16:311:LEU:CD1    | 2.03                     | 0.68              |
| 5:P16:402:LEU:HD13   | 5:P16:433:LEU:HD13   | 1.74                     | 0.68              |
| 9:K8:614:PHE:CA      | 9:K8:683:GLN:HE22    | 2.07                     | 0.68              |
| 9:K8:923:ILE:CG2     | 9:K8:929:ARG:NE      | 2.53                     | 0.68              |
| 9:K8:1065:GLU:O      | 9:K8:1067:VAL:N      | 2.26                     | 0.68              |
| 10:C16:453:LEU:CD1   | 10:C16:486:LEU:CD2   | 2.70                     | 0.68              |
| 11:A24:736:PRO:HB2   | 24:D16:871:ARG:NH1   | 2.08                     | 0.68              |
| 10:C24:300:VAL:CG1   | 10:C24:317:ARG:HG3   | 2.23                     | 0.68              |
| 10:C24:453:LEU:CD1   | 10:C24:486:LEU:CD2   | 2.70                     | 0.68              |
| 12:A:212:LYS:CE      | 12:A:585:MET:HE3     | 2.14                     | 0.68              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:586:PRO:HD2    | 10:C:650:ARG:HH11   | 1.54                     | 0.68              |
| 10:C:1280:VAL:HG22  | 10:C:1731:HIS:ND1   | 2.08                     | 0.68              |
| 11:A16:154:ILE:HD11 | 18:B:1842:VAL:CG1   | 2.20                     | 0.68              |
| 18:B:1006:VAL:HG21  | 18:B:1027:LEU:HD11  | 1.75                     | 0.68              |
| 18:B:1081:LEU:HD12  | 18:B:1337:SER:OG    | 1.94                     | 0.68              |
| 18:B:1175:ALA:HB1   | 18:B:1272:TRP:HD1   | 1.58                     | 0.68              |
| 18:B8:660:ALA:HB3   | 18:B8:661:PRO:HD3   | 1.76                     | 0.68              |
| 18:B8:1719:SER:HB3  | 18:B8:1720:PRO:HD3  | 1.74                     | 0.68              |
| 18:B8:1788:ILE:O    | 18:B8:1789:THR:C    | 2.27                     | 0.68              |
| 22:I8:333:ARG:HG3   | 22:I8:350:PHE:CE2   | 2.28                     | 0.68              |
| 12:A48:704:ILE:HG12 | 12:A48:760:LEU:HD12 | 1.75                     | 0.68              |
| 1:R:1115:TYR:HB2    | 1:R:1131:MET:CE     | 2.23                     | 0.68              |
| 2:M:417:ARG:NH1     | 8:L:299:ASP:HA      | 2.08                     | 0.68              |
| 1:R8:1379:GLN:NE2   | 1:R8:1416:TYR:HE1   | 1.92                     | 0.68              |
| 2:M8:202:LYS:NZ     | 2:M8:208:SER:N      | 2.39                     | 0.68              |
| 2:M8:669:ALA:HB1    | 2:M8:684:GLN:HG3    | 0.69                     | 0.68              |
| 2:M16:414:GLY:CA    | 8:L16:401:LYS:HZ3   | 1.98                     | 0.68              |
| 4:T16:671:ILE:HD11  | 5:P16:698:GLY:CA    | 2.23                     | 0.68              |
| 5:P:159:ILE:HD11    | 5:P:214:LEU:CB      | 2.22                     | 0.68              |
| 5:P8:458:GLU:OE1    | 5:P8:462:ARG:NH2    | 2.26                     | 0.68              |
| 8:L16:1096:GLU:OE1  | 9:K16:998:GLN:CD    | 2.36                     | 0.68              |
| 9:K:585:GLU:HA      | 9:K:622:VAL:CG1     | 2.23                     | 0.68              |
| 9:K:634:LEU:CD2     | 9:K:754:ARG:HH12    | 2.00                     | 0.68              |
| 9:K8:635:ALA:CB     | 9:K8:655:GLN:CD     | 2.63                     | 0.68              |
| 10:C24:1271:PHE:CZ  | 10:C24:1284:ASP:CB  | 2.74                     | 0.68              |
| 11:A40:103:GLU:HG2  | 21:H16:323:TYR:CE2  | 2.28                     | 0.68              |
| 10:C:26:ARG:HH21    | 10:C:151:LEU:HB2    | 1.58                     | 0.68              |
| 10:C8:1507:LEU:C    | 10:C8:1509:SER:H    | 2.02                     | 0.68              |
| 11:A32:90:PHE:CZ    | 18:B8:1788:ILE:CG2  | 2.65                     | 0.68              |
| 11:A32:437:LEU:HD11 | 11:A32:454:LYS:CE   | 2.23                     | 0.68              |
| 18:B8:1161:LEU:CD1  | 18:B8:1403:ILE:CG2  | 2.68                     | 0.68              |
| 20:E:165:ARG:NH1    | 20:E:173:ILE:HD11   | 2.09                     | 0.68              |
| 20:E8:350:GLU:HG2   | 20:E8:352:PHE:HE2   | 1.58                     | 0.68              |
| 21:H8:271:LEU:HD21  | 22:I8:254:ILE:CG2   | 2.24                     | 0.68              |
| 21:H24:228:LEU:CD2  | 23:J24:592:VAL:HG12 | 2.23                     | 0.68              |
| 10:C32:1258:LEU:HA  | 10:C32:1323:LEU:CD1 | 2.23                     | 0.68              |
| 2:M:349:ASP:C       | 2:M:351:ALA:N       | 2.52                     | 0.68              |
| 5:P:401:ARG:HH22    | 5:P:404:ILE:HG22    | 1.57                     | 0.68              |
| 5:P8:16:PHE:CE2     | 5:P8:461:HIS:NE2    | 2.62                     | 0.68              |
| 9:K8:614:PHE:HA     | 9:K8:683:GLN:HE22   | 1.58                     | 0.68              |
| 9:K8:649:MET:CB     | 9:K8:704:ARG:HH22   | 2.06                     | 0.68              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C16:390:HIS:HD2  | 10:C16:452:LEU:CD1   | 2.06                     | 0.68              |
| 10:C24:228:ARG:HH22 | 10:C24:277:SER:HB3   | 1.57                     | 0.68              |
| 10:C24:278:ARG:HH11 | 10:C24:287:SER:HB2   | 1.56                     | 0.68              |
| 10:C24:1278:ASP:OD2 | 21:H24:283:LYS:HA    | 1.94                     | 0.68              |
| 11:A40:437:LEU:HD11 | 11:A40:454:LYS:CE    | 2.23                     | 0.68              |
| 12:A:643:SER:HB2    | 12:A:663:LEU:HD22    | 1.75                     | 0.68              |
| 10:C:182:ASP:HB2    | 10:C:183:PRO:CD      | 2.23                     | 0.68              |
| 10:C8:182:ASP:HB2   | 10:C8:183:PRO:CD     | 2.23                     | 0.68              |
| 10:C8:499:LEU:CD2   | 10:C8:505:PHE:CZ     | 2.77                     | 0.68              |
| 11:A32:121:GLN:NE2  | 18:B8:1559:ALA:CA    | 2.52                     | 0.68              |
| 18:B:671:MET:CE     | 18:B:733:VAL:HA      | 2.24                     | 0.68              |
| 18:B8:786:ASP:OD1   | 24:D32:1066:VAL:CG2  | 2.39                     | 0.68              |
| 19:4:3:SER:OG       | 19:4:19:LEU:HD12     | 1.92                     | 0.68              |
| 21:H16:271:LEU:HD21 | 22:I16:254:ILE:CG2   | 2.24                     | 0.68              |
| 10:C32:668:ALA:N    | 10:C32:700:MET:HE1   | 2.08                     | 0.68              |
| 10:C32:1507:LEU:C   | 10:C32:1509:SER:H    | 2.02                     | 0.68              |
| 2:M:544:LEU:HD21    | 2:M:586:ALA:HB1      | 1.75                     | 0.68              |
| 1:R8:1059:ILE:HG22  | 24:D40:1435:ARG:HH12 | 1.59                     | 0.68              |
| 1:R16:1203:SER:O    | 1:R16:1205:ASP:N     | 2.26                     | 0.68              |
| 2:M16:571:TYR:HD1   | 2:M16:595:LEU:CD1    | 2.07                     | 0.68              |
| 9:K:1065:GLU:O      | 9:K:1067:VAL:N       | 2.26                     | 0.68              |
| 10:C16:499:LEU:CD2  | 10:C16:505:PHE:CZ    | 2.77                     | 0.68              |
| 10:C16:1271:PHE:CZ  | 10:C16:1284:ASP:CB   | 2.74                     | 0.68              |
| 11:A24:259:ILE:HG22 | 11:A24:276:LEU:HD22  | 1.75                     | 0.68              |
| 11:A24:437:LEU:HD11 | 11:A24:454:LYS:CE    | 2.23                     | 0.68              |
| 13:V:854:LEU:HD21   | 14:W:734:SER:HB3     | 1.74                     | 0.68              |
| 14:W:746:THR:HG21   | 15:J:675:ASN:HD21    | 1.56                     | 0.68              |
| 10:C:153:ALA:C      | 24:D:1403:LEU:HD11   | 2.19                     | 0.68              |
| 10:C:798:VAL:HG12   | 10:C:802:TRP:CE2     | 2.29                     | 0.68              |
| 10:C8:1280:VAL:HG22 | 10:C8:1731:HIS:ND1   | 2.08                     | 0.68              |
| 11:A16:845:THR:OG1  | 24:D16:1297:HIS:HE1  | 1.76                     | 0.68              |
| 17:F16:73:GLY:O     | 17:F16:75:ALA:N      | 2.25                     | 0.68              |
| 18:B:191:PHE:CD2    | 18:B:192:PRO:O       | 2.47                     | 0.68              |
| 18:B:1112:LYS:NZ    | 21:H:327:SER:C       | 2.51                     | 0.68              |
| 18:B8:1110:LEU:HD21 | 21:H24:326:GLY:CA    | 2.22                     | 0.68              |
| 18:B8:1856:PHE:CZ   | 18:B8:1916:VAL:HG21  | 2.28                     | 0.68              |
| 21:H8:280:LEU:HD21  | 22:I8:262:LEU:HG     | 1.74                     | 0.68              |
| 22:I16:333:ARG:HG3  | 22:I16:350:PHE:CE2   | 2.28                     | 0.68              |
| 24:D:403:ARG:CD     | 24:D16:744:LEU:O     | 2.41                     | 0.68              |
| 10:C32:499:LEU:CD2  | 10:C32:505:PHE:CZ    | 2.77                     | 0.68              |
| 12:A48:707:LEU:HD21 | 12:A48:767:ARG:HH22  | 1.59                     | 0.68              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R:1203:SER:O      | 1:R:1205:ASP:N       | 2.26                     | 0.68              |
| 2:M:210:GLN:OE1     | 10:C:529:GLN:NE2     | 2.26                     | 0.68              |
| 2:M:625:HIS:CD2     | 3:N:225:PRO:HA       | 2.27                     | 0.68              |
| 1:R16:1168:LEU:HD23 | 1:R16:1216:ILE:CG1   | 2.24                     | 0.68              |
| 7:Q16:98:MET:CE     | 7:Q16:110:VAL:CG1    | 2.71                     | 0.68              |
| 8:L:1041:SER:OG     | 8:L:1054:HIS:CE1     | 2.39                     | 0.68              |
| 8:L:1077:LEU:CD1    | 9:K:1086:VAL:HG12    | 2.17                     | 0.68              |
| 9:K:806:LEU:CD1     | 9:K:874:VAL:CG1      | 2.72                     | 0.68              |
| 9:K8:806:LEU:CD1    | 9:K8:874:VAL:CG1     | 2.72                     | 0.68              |
| 10:C16:668:ALA:N    | 10:C16:700:MET:HE1   | 2.08                     | 0.68              |
| 10:C16:795:ASP:OD2  | 10:C16:850:ARG:NH1   | 2.25                     | 0.68              |
| 10:C16:1258:LEU:HA  | 10:C16:1323:LEU:CD1  | 2.23                     | 0.68              |
| 11:A24:72:ILE:CD1   | 21:H8:348:ALA:HA     | 2.24                     | 0.68              |
| 11:A24:326:TYR:OH   | 17:F:74:ILE:O        | 2.12                     | 0.68              |
| 10:C24:168:ARG:HH11 | 10:C24:229:PRO:HA    | 1.57                     | 0.68              |
| 10:C24:1258:LEU:HA  | 10:C24:1323:LEU:CD1  | 2.23                     | 0.68              |
| 10:C:1766:ILE:HD13  | 10:C:1800:LEU:HD21   | 1.74                     | 0.68              |
| 10:C8:1158:HIS:CE1  | 10:C8:1164:VAL:HG11  | 2.28                     | 0.68              |
| 10:C8:1271:PHE:HE2  | 10:C8:1284:ASP:CB    | 2.06                     | 0.68              |
| 11:A16:72:ILE:CD1   | 21:H:348:ALA:HA      | 2.24                     | 0.68              |
| 11:A32:440:LEU:HD12 | 11:A32:443:LEU:HD11  | 1.75                     | 0.68              |
| 18:B:1575:GLN:HE21  | 24:D16:1403:LEU:HD23 | 0.51                     | 0.68              |
| 18:B8:671:MET:CE    | 18:B8:733:VAL:HA     | 2.24                     | 0.68              |
| 18:B8:1081:LEU:HD12 | 18:B8:1337:SER:OG    | 1.94                     | 0.68              |
| 19:48:3:SER:OG      | 19:48:19:LEU:HD12    | 1.93                     | 0.68              |
| 19:48:281:TRP:CD2   | 19:48:288:SER:HB3    | 2.29                     | 0.68              |
| 21:H24:316:ILE:O    | 21:H24:317:ALA:C     | 2.35                     | 0.68              |
| 24:D:44:SER:HB3     | 24:D16:761:ASN:ND2   | 2.09                     | 0.68              |
| 10:C32:1158:HIS:CE1 | 10:C32:1164:VAL:HG11 | 2.28                     | 0.68              |
| 1:R:1441:TYR:CE2    | 2:M:181:LEU:HG       | 2.29                     | 0.68              |
| 2:M:182:PHE:CE2     | 3:N:214:ARG:NH1      | 2.62                     | 0.68              |
| 2:M:571:TYR:HD1     | 2:M:595:LEU:CD1      | 2.07                     | 0.68              |
| 3:N:15:HIS:HE2      | 3:N:31:SER:HG        | 1.42                     | 0.68              |
| 1:R8:983:ARG:NH1    | 24:D40:1364:PRO:O    | 2.27                     | 0.68              |
| 1:R16:1269:LEU:HD12 | 5:P16:684:ARG:HE     | 1.55                     | 0.68              |
| 1:R16:1441:TYR:CE2  | 2:M16:181:LEU:HG     | 2.29                     | 0.68              |
| 2:M16:819:GLN:OE1   | 2:M16:846:LEU:HD21   | 1.92                     | 0.68              |
| 5:P:303:LYS:CE      | 14:W:84:PRO:O        | 2.34                     | 0.68              |
| 7:Q8:297:VAL:HG13   | 7:Q8:301:ARG:CD      | 2.23                     | 0.68              |
| 5:P16:207:HIS:HB3   | 5:P16:208:PRO:HD2    | 1.74                     | 0.68              |
| 10:C16:1251:PHE:HZ  | 10:C16:1319:ARG:CZ   | 1.99                     | 0.68              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1280:VAL:HG22 | 10:C16:1731:HIS:ND1  | 2.08                     | 0.68              |
| 10:C24:499:LEU:CD2   | 10:C24:505:PHE:CZ    | 2.77                     | 0.68              |
| 10:C24:798:VAL:HG12  | 10:C24:802:TRP:CE2   | 2.29                     | 0.68              |
| 10:C24:1477:GLN:NE2  | 24:D24:1407:PHE:CD1  | 2.62                     | 0.68              |
| 11:A40:437:LEU:HD11  | 11:A40:454:LYS:HZ3   | 1.57                     | 0.68              |
| 12:A:225:ARG:HH11    | 12:A:228:MET:HE1     | 1.56                     | 0.68              |
| 12:A:259:ILE:HG22    | 12:A:276:LEU:HD22    | 1.75                     | 0.68              |
| 14:W:1:MET:HE2       | 10:C:1497:LYS:CD     | 2.15                     | 0.68              |
| 10:C8:513:LEU:HD13   | 10:C8:549:TYR:HB3    | 1.76                     | 0.68              |
| 10:C8:792:PHE:HD1    | 10:C8:850:ARG:NH1    | 1.92                     | 0.68              |
| 10:C8:798:VAL:HG12   | 10:C8:802:TRP:CE2    | 2.29                     | 0.68              |
| 10:C8:1258:LEU:HA    | 10:C8:1323:LEU:CD1   | 2.23                     | 0.68              |
| 18:B:349:PHE:CZ      | 18:B:353:ILE:CD1     | 2.59                     | 0.68              |
| 18:B:638:ALA:HA      | 18:B:699:MET:HE3     | 1.76                     | 0.68              |
| 18:B8:113:TYR:HE1    | 18:B8:119:VAL:HG11   | 1.57                     | 0.68              |
| 18:B8:514:THR:HG22   | 18:B8:549:TRP:HH2    | 1.58                     | 0.68              |
| 18:B8:683:ASN:C      | 18:B8:685:SER:H      | 2.01                     | 0.68              |
| 18:B8:1006:VAL:HG21  | 18:B8:1027:LEU:HD11  | 1.75                     | 0.68              |
| 19:4:100:ILE:CD1     | 19:4:274:PHE:CE1     | 2.76                     | 0.68              |
| 19:4:153:ARG:CZ      | 20:E:467:ILE:HD11    | 2.24                     | 0.68              |
| 21:H24:322:LEU:HD13  | 23:J24:689:LEU:HG    | 1.75                     | 0.68              |
| 21:H16:228:LEU:CD2   | 23:J16:592:VAL:HG12  | 2.23                     | 0.68              |
| 21:H16:322:LEU:HD13  | 23:J16:689:LEU:HG    | 1.75                     | 0.68              |
| 10:C32:795:ASP:OD2   | 10:C32:850:ARG:NH1   | 2.25                     | 0.68              |
| 10:C32:1352:GLN:CD   | 10:C32:1357:LEU:HD12 | 2.18                     | 0.68              |
| 10:C32:1593:TRP:CZ2  | 10:C32:1603:PHE:CD2  | 2.82                     | 0.68              |
| 2:M:202:LYS:NZ       | 2:M:208:SER:C        | 2.49                     | 0.68              |
| 1:R8:1266:THR:CB     | 5:P8:684:ARG:NH2     | 2.56                     | 0.68              |
| 2:M8:202:LYS:NZ      | 2:M8:208:SER:C       | 2.49                     | 0.68              |
| 3:N8:267:TRP:CH2     | 3:N8:294:TRP:HH2     | 2.12                     | 0.68              |
| 2:M16:202:LYS:NZ     | 2:M16:208:SER:N      | 2.39                     | 0.68              |
| 5:P:16:PHE:CE2       | 5:P:461:HIS:NE2      | 2.61                     | 0.68              |
| 7:Q:98:MET:CE        | 7:Q:110:VAL:CG1      | 2.71                     | 0.68              |
| 8:L8:1096:GLU:CD     | 9:K8:996:MET:HB3     | 2.17                     | 0.68              |
| 9:K8:707:GLN:NE2     | 9:K8:734:TRP:HE3     | 1.92                     | 0.68              |
| 9:K8:869:GLU:OE1     | 9:K8:944:ASN:CB      | 2.39                     | 0.68              |
| 14:W:642:LEU:HD21    | 15:J:568:ILE:HD13    | 1.75                     | 0.68              |
| 10:C:1258:LEU:HA     | 10:C:1323:LEU:CD1    | 2.23                     | 0.68              |
| 10:C8:26:ARG:HH21    | 10:C8:151:LEU:HB2    | 1.58                     | 0.68              |
| 10:C8:960:PHE:CE1    | 10:C8:1138:GLU:CB    | 2.77                     | 0.68              |
| 11:A32:154:ILE:HD11  | 18:B8:1842:VAL:CG1   | 2.20                     | 0.68              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B:1856:PHE:CZ    | 18:B:1916:VAL:HG21   | 2.28                     | 0.68              |
| 18:B8:86:LYS:HE2    | 18:B8:123:LEU:HD12   | 1.75                     | 0.68              |
| 18:B8:1342:LEU:CD2  | 18:B8:1406:ALA:CB    | 2.69                     | 0.68              |
| 18:B8:1783:VAL:CG2  | 18:B8:1810:VAL:HG11  | 2.24                     | 0.68              |
| 18:B8:1793:ILE:O    | 18:B8:1794:SER:C     | 2.29                     | 0.68              |
| 18:B8:1802:ASP:C    | 18:B8:1804:THR:N     | 2.52                     | 0.68              |
| 24:D:405:GLN:CB     | 24:D16:10:ARG:NH1    | 2.40                     | 0.68              |
| 10:C32:792:PHE:HD1  | 10:C32:850:ARG:NH1   | 1.92                     | 0.68              |
| 1:R8:1441:TYR:CE2   | 2:M8:181:LEU:HG      | 2.29                     | 0.68              |
| 3:N16:15:HIS:HE2    | 3:N16:31:SER:HG      | 1.40                     | 0.68              |
| 5:P:633:LEU:C       | 5:P:633:LEU:HD23     | 2.19                     | 0.68              |
| 5:P8:504:GLN:NE2    | 6:O8:22:ASP:OD2      | 2.27                     | 0.68              |
| 8:L8:608:PHE:CE1    | 8:L8:635:MET:HA      | 2.29                     | 0.68              |
| 8:L8:1041:SER:OG    | 8:L8:1054:HIS:CE1    | 2.39                     | 0.68              |
| 8:L16:605:MET:SD    | 8:L16:631:LEU:HD13   | 2.31                     | 0.68              |
| 9:K8:703:LEU:HD13   | 9:K8:805:ILE:HD11    | 1.74                     | 0.68              |
| 10:C16:168:ARG:NH1  | 10:C16:229:PRO:CA    | 2.57                     | 0.68              |
| 10:C16:792:PHE:HD1  | 10:C16:850:ARG:NH1   | 1.92                     | 0.68              |
| 10:C16:847:ARG:CZ   | 10:C16:911:ILE:N     | 2.57                     | 0.68              |
| 10:C16:1068:THR:O   | 10:C16:1069:TYR:C    | 2.25                     | 0.68              |
| 10:C16:1158:HIS:CE1 | 10:C16:1164:VAL:HG11 | 2.28                     | 0.68              |
| 10:C16:1274:ALA:C   | 10:C16:1276:SER:N    | 2.48                     | 0.68              |
| 11:A24:468:VAL:HG11 | 24:D16:1100:GLN:HB3  | 1.76                     | 0.68              |
| 11:A24:803:PRO:CA   | 24:D8:1401:LEU:HD12  | 2.24                     | 0.68              |
| 10:C24:668:ALA:N    | 10:C24:700:MET:HE1   | 2.08                     | 0.68              |
| 10:C24:848:CYS:CA   | 10:C24:906:ARG:HH22  | 1.97                     | 0.68              |
| 11:A40:198:PRO:HB2  | 11:A40:200:HIS:ND1   | 2.09                     | 0.68              |
| 14:W:638:VAL:HG11   | 15:J:561:PHE:HE2     | 1.51                     | 0.68              |
| 15:J:591:LYS:O      | 15:J:595:THR:OG1     | 2.12                     | 0.68              |
| 10:C:1023:LEU:HD22  | 10:C:1210:ILE:HD12   | 1.76                     | 0.68              |
| 10:C:1265:ARG:C     | 10:C:1268:ARG:HE     | 2.02                     | 0.68              |
| 10:C:1265:ARG:C     | 10:C:1268:ARG:HG2    | 2.19                     | 0.68              |
| 10:C8:228:ARG:HH22  | 10:C8:277:SER:HB3    | 1.57                     | 0.68              |
| 10:C8:1274:ALA:C    | 10:C8:1276:SER:N     | 2.48                     | 0.68              |
| 11:A32:704:ILE:HG12 | 11:A32:760:LEU:HD12  | 1.75                     | 0.68              |
| 18:B:86:LYS:HE2     | 18:B:123:LEU:HD12    | 1.75                     | 0.68              |
| 18:B:111:GLN:OE1    | 18:B:134:GLN:NE2     | 2.25                     | 0.68              |
| 18:B8:94:LEU:HD21   | 18:B8:132:LEU:HD22   | 1.74                     | 0.68              |
| 18:B8:266:ARG:NH1   | 18:B8:383:PHE:CB     | 2.57                     | 0.68              |
| 18:B8:729:LEU:HB2   | 18:B8:1196:MET:HE3   | 1.73                     | 0.68              |
| 21:H:228:LEU:CD2    | 23:J32:592:VAL:HG12  | 2.23                     | 0.68              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:453:LEU:CD1   | 10:C32:486:LEU:CD2   | 2.70                     | 0.68              |
| 2:M:363:ARG:HH12     | 2:M:494:SER:HB2      | 1.59                     | 0.67              |
| 3:N:267:TRP:CH2      | 3:N:294:TRP:HH2      | 2.12                     | 0.67              |
| 1:R8:1168:LEU:HD23   | 1:R8:1216:ILE:CG1    | 2.24                     | 0.67              |
| 2:M8:786:ARG:HG3     | 8:L16:472:GLU:OE1    | 1.93                     | 0.67              |
| 2:M16:349:ASP:C      | 2:M16:351:ALA:N      | 2.52                     | 0.67              |
| 2:M16:672:TYR:CZ     | 2:M16:680:LYS:NZ     | 2.48                     | 0.67              |
| 5:P16:504:GLN:NE2    | 6:O16:22:ASP:OD2     | 2.27                     | 0.67              |
| 9:K:614:PHE:HA       | 9:K:683:GLN:HE22     | 1.58                     | 0.67              |
| 9:K:707:GLN:NE2      | 9:K:734:TRP:HE3      | 1.92                     | 0.67              |
| 10:C16:1023:LEU:HD22 | 10:C16:1210:ILE:HD12 | 1.76                     | 0.67              |
| 11:A24:56:ALA:C      | 11:A24:58:SER:N      | 2.49                     | 0.67              |
| 11:A24:198:PRO:HB2   | 11:A24:200:HIS:ND1   | 2.09                     | 0.67              |
| 11:A24:468:VAL:HG21  | 24:D16:1100:GLN:CG   | 2.25                     | 0.67              |
| 10:C24:1158:HIS:CE1  | 10:C24:1164:VAL:HG11 | 2.28                     | 0.67              |
| 10:C24:1488:ILE:HD11 | 10:C24:1528:LEU:HD23 | 1.76                     | 0.67              |
| 10:C24:1716:LYS:HG3  | 10:C24:1721:GLN:NE2  | 2.07                     | 0.67              |
| 11:A40:259:ILE:HG22  | 11:A40:276:LEU:HD22  | 1.75                     | 0.67              |
| 10:C:281:ASP:CB      | 24:D:1398:ARG:HG3    | 2.24                     | 0.67              |
| 10:C:513:LEU:HD13    | 10:C:549:TYR:HB3     | 1.76                     | 0.67              |
| 10:C:565:ARG:CZ      | 10:C:569:PHE:CD2     | 2.67                     | 0.67              |
| 10:C:1274:ALA:C      | 10:C:1276:SER:N      | 2.48                     | 0.67              |
| 10:C8:1023:LEU:HD22  | 10:C8:1210:ILE:HD12  | 1.76                     | 0.67              |
| 10:C8:1033:GLY:C     | 10:C8:1218:ARG:HH22  | 2.01                     | 0.67              |
| 10:C8:1622:SER:OG    | 10:C8:1623:ILE:N     | 2.08                     | 0.67              |
| 11:A16:704:ILE:HG12  | 11:A16:760:LEU:HD12  | 1.75                     | 0.67              |
| 11:A32:51:THR:HG23   | 22:I24:317:HIS:HB2   | 1.74                     | 0.67              |
| 11:A32:198:PRO:HB2   | 11:A32:200:HIS:ND1   | 2.09                     | 0.67              |
| 11:A32:714:GLY:HA2   | 24:D32:1398:ARG:NH2  | 2.08                     | 0.67              |
| 18:B:856:LEU:HD23    | 18:B:860:HIS:HB2     | 1.75                     | 0.67              |
| 19:48:51:PRO:O       | 19:48:53:SER:N       | 2.27                     | 0.67              |
| 21:H:322:LEU:HD13    | 23:J32:689:LEU:HG    | 1.75                     | 0.67              |
| 22:I8:131:ARG:HE     | 23:J8:557:ARG:NH2    | 1.91                     | 0.67              |
| 21:H24:228:LEU:HD21  | 23:J24:592:VAL:HG12  | 1.76                     | 0.67              |
| 21:H24:271:LEU:HD21  | 22:I24:254:ILE:CG2   | 2.24                     | 0.67              |
| 22:I24:333:ARG:HG3   | 22:I24:350:PHE:CE2   | 2.29                     | 0.67              |
| 1:R:1326:GLY:HA3     | 10:C:1154:TRP:CZ2    | 2.30                     | 0.67              |
| 1:R:1360:GLN:O       | 10:C:608:ASP:HB2     | 1.93                     | 0.67              |
| 2:M16:202:LYS:NZ     | 2:M16:208:SER:C      | 2.49                     | 0.67              |
| 3:N16:267:TRP:CH2    | 3:N16:294:TRP:HH2    | 2.12                     | 0.67              |
| 9:K16:792:LEU:CD1    | 9:K16:864:ILE:HD11   | 2.24                     | 0.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1166:SER:O    | 10:C16:1168:PRO:N    | 2.24                     | 0.67              |
| 10:C16:1265:ARG:C    | 10:C16:1268:ARG:HE   | 2.02                     | 0.67              |
| 10:C16:1547:LYS:HD2  | 24:D8:1406:SER:HB2   | 1.77                     | 0.67              |
| 11:A24:307:GLY:HA3   | 20:E:387:LEU:HD21    | 1.76                     | 0.67              |
| 10:C24:1023:LEU:HD22 | 10:C24:1210:ILE:HD12 | 1.76                     | 0.67              |
| 10:C24:1265:ARG:C    | 10:C24:1268:ARG:HE   | 2.02                     | 0.67              |
| 10:C24:1777:SER:O    | 10:C24:1778:ASN:C    | 2.26                     | 0.67              |
| 11:A40:72:ILE:CD1    | 21:H16:348:ALA:HA    | 2.24                     | 0.67              |
| 12:A:707:LEU:HD21    | 12:A:767:ARG:HH22    | 1.59                     | 0.67              |
| 13:V:745:LEU:HD11    | 15:J:557:ARG:HH11    | 1.58                     | 0.67              |
| 15:J:658:LEU:HD23    | 15:J:661:MET:HE3     | 1.76                     | 0.67              |
| 10:C:57:VAL:HA       | 10:C:62:ILE:HD11     | 1.77                     | 0.67              |
| 10:C:1507:LEU:C      | 10:C:1509:SER:H      | 2.02                     | 0.67              |
| 11:A32:121:GLN:HE22  | 18:B8:1559:ALA:HB1   | 1.57                     | 0.67              |
| 18:B:266:ARG:NH1     | 18:B:383:PHE:CB      | 2.57                     | 0.67              |
| 18:B:842:ASN:OD1     | 18:B:899:LYS:HE3     | 1.94                     | 0.67              |
| 18:B8:904:ALA:CB     | 18:B8:917:PHE:HZ     | 2.08                     | 0.67              |
| 20:E:33:PHE:HD1      | 20:E:37:LEU:HD12     | 1.58                     | 0.67              |
| 21:H:228:LEU:HD21    | 23:J32:592:VAL:HG12  | 1.76                     | 0.67              |
| 21:H:271:LEU:HD21    | 22:I:254:ILE:CG2     | 2.23                     | 0.67              |
| 21:H8:215:ARG:O      | 21:H8:218:ILE:HG22   | 1.95                     | 0.67              |
| 22:I24:203:GLN:HB3   | 22:I24:209:TRP:CH2   | 2.30                     | 0.67              |
| 10:C32:1023:LEU:HD22 | 10:C32:1210:ILE:HD12 | 1.76                     | 0.67              |
| 1:R:1033:LYS:HZ3     | 24:D:1432:THR:HG21   | 1.58                     | 0.67              |
| 1:R:1324:ASP:CG      | 10:C:1180:ILE:CB     | 2.67                     | 0.67              |
| 1:R:1379:GLN:NE2     | 1:R:1416:TYR:HE1     | 1.92                     | 0.67              |
| 2:M:420:CYS:HB3      | 8:L:391:TRP:CH2      | 2.28                     | 0.67              |
| 3:N:162:THR:HG22     | 3:N:168:VAL:HG22     | 1.75                     | 0.67              |
| 2:M8:182:PHE:CE2     | 3:N8:214:ARG:NH1     | 2.62                     | 0.67              |
| 2:M8:540:TYR:CE1     | 2:M8:555:LEU:HD23    | 2.29                     | 0.67              |
| 1:R16:1165:MET:HE1   | 1:R16:1220:GLN:HG2   | 1.76                     | 0.67              |
| 1:R16:1228:ALA:HB2   | 1:R16:1263:MET:HE2   | 1.75                     | 0.67              |
| 2:M16:162:ILE:HD11   | 2:M16:213:LEU:CD1    | 2.24                     | 0.67              |
| 2:M16:182:PHE:CE2    | 3:N16:214:ARG:NH1    | 2.62                     | 0.67              |
| 2:M16:571:TYR:CD1    | 2:M16:595:LEU:CD1    | 2.78                     | 0.67              |
| 5:P:633:LEU:HD21     | 5:P:639:THR:CG2      | 2.23                     | 0.67              |
| 5:P8:207:HIS:HB3     | 5:P8:208:PRO:HD2     | 1.74                     | 0.67              |
| 9:K:614:PHE:CA       | 9:K:683:GLN:HE22     | 2.06                     | 0.67              |
| 9:K:1071:PHE:CZ      | 9:K:1107:LEU:HD23    | 2.30                     | 0.67              |
| 9:K8:585:GLU:HA      | 9:K8:622:VAL:CG1     | 2.23                     | 0.67              |
| 9:K8:1142:ARG:NH2    | 9:K8:1204:THR:CA     | 2.56                     | 0.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:668:ALA:HA    | 10:C24:700:MET:HE3   | 1.76                     | 0.67              |
| 10:C:792:PHE:HD1     | 10:C:850:ARG:NH1     | 1.92                     | 0.67              |
| 10:C8:1265:ARG:C     | 10:C8:1268:ARG:HE    | 2.02                     | 0.67              |
| 10:C8:1333:HIS:CE1   | 10:C8:1337:LEU:CD2   | 2.78                     | 0.67              |
| 11:A16:703:ALA:CB    | 24:D16:1398:ARG:HH11 | 2.06                     | 0.67              |
| 11:A32:496:LYS:NZ    | 17:F24:64:ASP:OD2    | 2.26                     | 0.67              |
| 18:B8:842:ASN:OD1    | 18:B8:899:LYS:HE3    | 1.94                     | 0.67              |
| 18:B8:1065:LYS:O     | 18:B8:1067:SER:N     | 2.25                     | 0.67              |
| 19:4:183:ARG:NH1     | 19:4:245:GLY:CA      | 2.32                     | 0.67              |
| 19:4:281:TRP:CD2     | 19:4:288:SER:HB3     | 2.29                     | 0.67              |
| 22:I:333:ARG:HG3     | 22:I:350:PHE:CE2     | 2.28                     | 0.67              |
| 10:C32:168:ARG:HH11  | 10:C32:229:PRO:HA    | 1.56                     | 0.67              |
| 10:C32:228:ARG:HH22  | 10:C32:277:SER:HB3   | 1.57                     | 0.67              |
| 10:C32:1624:LEU:HD21 | 10:C32:1632:LEU:HD11 | 1.77                     | 0.67              |
| 1:R:1191:LYS:HD2     | 24:D:1453:GLU:OE1    | 1.93                     | 0.67              |
| 1:R:1449:TRP:HH2     | 2:M:161:ASP:O        | 1.76                     | 0.67              |
| 1:R8:1165:MET:HE1    | 1:R8:1220:GLN:HG2    | 1.77                     | 0.67              |
| 2:M8:328:THR:HG21    | 2:M8:350:SER:OG      | 1.93                     | 0.67              |
| 2:M8:571:TYR:HD1     | 2:M8:595:LEU:CD1     | 2.06                     | 0.67              |
| 5:P:187:TRP:CZ3      | 5:P:191:ARG:HG2      | 2.30                     | 0.67              |
| 9:K:578:THR:CG2      | 9:K:616:ARG:HH21     | 1.85                     | 0.67              |
| 10:C16:168:ARG:HH11  | 10:C16:229:PRO:HA    | 1.56                     | 0.67              |
| 10:C16:798:VAL:HG12  | 10:C16:802:TRP:CE2   | 2.29                     | 0.67              |
| 11:A40:704:ILE:HG12  | 11:A40:760:LEU:HD12  | 1.75                     | 0.67              |
| 11:A32:148:LEU:CD1   | 18:B8:1956:ILE:HD12  | 2.24                     | 0.67              |
| 18:B:849:SER:O       | 18:B:852:THR:HG23    | 1.94                     | 0.67              |
| 18:B:1045:LYS:HZ1    | 18:B:1100:LEU:HD21   | 1.60                     | 0.67              |
| 18:B:1390:LEU:CD1    | 18:B:1404:LEU:HD11   | 2.25                     | 0.67              |
| 18:B:1768:ILE:CD1    | 18:B:1895:LEU:HD22   | 2.25                     | 0.67              |
| 18:B:1802:ASP:C      | 18:B:1804:THR:N      | 2.52                     | 0.67              |
| 18:B8:191:PHE:CD2    | 18:B8:192:PRO:O      | 2.47                     | 0.67              |
| 18:B8:712:PRO:HB3    | 18:B8:759:MET:HE2    | 1.75                     | 0.67              |
| 18:B8:728:GLY:O      | 18:B8:1197:VAL:HG23  | 1.95                     | 0.67              |
| 18:B8:968:PHE:HB2    | 18:B8:1040:MET:HE1   | 1.76                     | 0.67              |
| 20:E:350:GLU:HG2     | 20:E:352:PHE:HE2     | 1.58                     | 0.67              |
| 10:C32:508:ILE:HG23  | 10:C32:549:TYR:OH    | 1.95                     | 0.67              |
| 10:C32:1280:VAL:HG22 | 10:C32:1731:HIS:ND1  | 2.08                     | 0.67              |
| 1:R:1428:VAL:HG23    | 6:O:165:LYS:HE2      | 1.75                     | 0.67              |
| 2:M:571:TYR:CD1      | 2:M:595:LEU:CD1      | 2.78                     | 0.67              |
| 2:M16:408:GLU:CG     | 8:L16:484:PRO:HG3    | 2.24                     | 0.67              |
| 5:P8:187:TRP:CZ3     | 5:P8:191:ARG:HG2     | 2.30                     | 0.67              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:K8:751:LEU:CD2    | 9:K8:754:ARG:HD3    | 2.25                     | 0.67              |
| 11:A24:704:ILE:HG12 | 11:A24:760:LEU:HD12 | 1.75                     | 0.67              |
| 10:C24:57:VAL:HA    | 10:C24:62:ILE:HD11  | 1.77                     | 0.67              |
| 10:C24:513:LEU:HD13 | 10:C24:549:TYR:HB3  | 1.76                     | 0.67              |
| 10:C24:717:GLU:OE1  | 23:J16:656:ARG:HD3  | 1.93                     | 0.67              |
| 10:C:499:LEU:CD2    | 10:C:505:PHE:CZ     | 2.77                     | 0.67              |
| 10:C:1271:PHE:CZ    | 10:C:1284:ASP:CB    | 2.74                     | 0.67              |
| 11:A16:198:PRO:HB2  | 11:A16:200:HIS:ND1  | 2.09                     | 0.67              |
| 11:A32:56:ALA:C     | 11:A32:58:SER:N     | 2.49                     | 0.67              |
| 18:B:94:LEU:HD21    | 18:B:132:LEU:HD22   | 1.74                     | 0.67              |
| 18:B:1783:VAL:CG2   | 18:B:1810:VAL:HG11  | 2.24                     | 0.67              |
| 18:B8:789:LEU:CD2   | 18:B8:793:LEU:HD12  | 2.19                     | 0.67              |
| 18:B8:849:SER:O     | 18:B8:852:THR:HG23  | 1.94                     | 0.67              |
| 19:4:51:PRO:O       | 19:4:53:SER:N       | 2.27                     | 0.67              |
| 20:E8:165:ARG:NH1   | 20:E8:173:ILE:HD11  | 2.09                     | 0.67              |
| 21:H8:322:LEU:HD13  | 23:J8:689:LEU:HG    | 1.76                     | 0.67              |
| 22:I24:289:LEU:CD2  | 22:I24:296:ARG:HH22 | 2.07                     | 0.67              |
| 22:I16:203:GLN:HB3  | 22:I16:209:TRP:CH2  | 2.30                     | 0.67              |
| 1:R:979:GLN:OE1     | 24:D:1438:ALA:CB    | 2.42                     | 0.67              |
| 1:R:1334:GLU:HB3    | 10:C:1170:VAL:CG2   | 2.24                     | 0.67              |
| 1:R16:1078:SER:OG   | 5:P16:713:LEU:HD22  | 1.92                     | 0.67              |
| 1:R16:1139:ARG:HG3  | 1:R16:1157:ARG:HH12 | 1.59                     | 0.67              |
| 1:R16:1449:TRP:HH2  | 2:M16:161:ASP:O     | 1.76                     | 0.67              |
| 9:K:1085:TYR:CE1    | 9:K:1093:SER:C      | 2.70                     | 0.67              |
| 9:K8:806:LEU:HD13   | 9:K8:874:VAL:HG12   | 1.74                     | 0.67              |
| 10:C16:1290:HIS:HB2 | 10:C16:1334:MET:CE  | 2.25                     | 0.67              |
| 10:C16:1547:LYS:HZ3 | 24:D8:1405:GLY:C    | 2.02                     | 0.67              |
| 10:C24:795:ASP:OD2  | 10:C24:850:ARG:NH1  | 2.25                     | 0.67              |
| 12:A:156:MET:CE     | 10:C8:58:GLN:O      | 2.28                     | 0.67              |
| 13:V:808:LYS:HE3    | 15:J:616:ALA:CB     | 2.24                     | 0.67              |
| 10:C:668:ALA:HA     | 10:C:700:MET:HE3    | 1.76                     | 0.67              |
| 10:C8:643:LEU:HD21  | 10:C8:656:THR:CG2   | 2.25                     | 0.67              |
| 18:B8:676:ASP:O     | 18:B8:678:PRO:CD    | 2.40                     | 0.67              |
| 18:B8:1768:ILE:CD1  | 18:B8:1895:LEU:HD22 | 2.25                     | 0.67              |
| 19:48:293:LEU:CD1   | 19:48:316:PHE:CE1   | 2.78                     | 0.67              |
| 21:H8:228:LEU:CD2   | 23:J8:592:VAL:HG12  | 2.23                     | 0.67              |
| 22:I16:131:ARG:HE   | 23:J16:557:ARG:NH2  | 1.91                     | 0.67              |
| 1:R:1063:ARG:HE     | 24:D:1432:THR:CG2   | 2.08                     | 0.67              |
| 1:R:1188:TYR:OH     | 24:D:1459:LEU:HD13  | 1.95                     | 0.67              |
| 1:R:1191:LYS:O      | 1:R:1192:LYS:C      | 2.35                     | 0.67              |
| 2:M:627:TYR:CE2     | 3:N:165:GLY:C       | 2.69                     | 0.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R8:1059:ILE:HG22   | 24:D40:1435:ARG:NH1  | 2.09                     | 0.67              |
| 1:R8:1228:ALA:HB2    | 1:R8:1263:MET:HE2    | 1.75                     | 0.67              |
| 2:M8:349:ASP:C       | 2:M8:351:ALA:N       | 2.52                     | 0.67              |
| 7:Q8:98:MET:CE       | 7:Q8:110:VAL:CG1     | 2.71                     | 0.67              |
| 9:K8:614:PHE:CA      | 9:K8:683:GLN:NE2     | 2.58                     | 0.67              |
| 11:A24:468:VAL:HG21  | 24:D16:1103:LEU:HD12 | 1.66                     | 0.67              |
| 13:V:814:MET:CE      | 13:V:824:TRP:CH2     | 2.77                     | 0.67              |
| 14:W:642:LEU:CD2     | 15:J:568:ILE:HD13    | 2.25                     | 0.67              |
| 14:W:688:HIS:CE1     | 14:W:692:GLU:OE2     | 2.48                     | 0.67              |
| 10:C:1068:THR:O      | 10:C:1069:TYR:C      | 2.25                     | 0.67              |
| 10:C8:1265:ARG:C     | 10:C8:1268:ARG:HG2   | 2.19                     | 0.67              |
| 11:A32:36:ASN:ND2    | 22:I24:293:LYS:HZ1   | 1.92                     | 0.67              |
| 18:B:1065:LYS:O      | 18:B:1067:SER:N      | 2.26                     | 0.67              |
| 18:B:1215:PHE:HE1    | 18:B:1234:MET:SD     | 2.13                     | 0.67              |
| 18:B8:457:SER:CA     | 18:B8:548:ARG:NH1    | 2.50                     | 0.67              |
| 18:B8:1768:ILE:HD13  | 18:B8:1895:LEU:CD2   | 2.24                     | 0.67              |
| 18:B8:1911:LEU:HD13  | 18:B8:1960:LEU:HD12  | 1.77                     | 0.67              |
| 19:4:293:LEU:CD1     | 19:4:316:PHE:CE1     | 2.77                     | 0.67              |
| 20:E:235:HIS:NE2     | 20:E:239:LYS:CE      | 2.55                     | 0.67              |
| 21:H8:291:VAL:CG1    | 23:J8:657:GLU:HG3    | 2.21                     | 0.67              |
| 1:R:1191:LYS:HB3     | 24:D:1453:GLU:OE1    | 1.93                     | 0.67              |
| 1:R8:1185:THR:CG2    | 24:D40:1462:PHE:CE2  | 2.77                     | 0.67              |
| 2:M16:349:ASP:O      | 2:M16:351:ALA:N      | 2.28                     | 0.67              |
| 3:N16:162:THR:HG22   | 3:N16:168:VAL:HG22   | 1.75                     | 0.67              |
| 5:P:207:HIS:CD2      | 5:P:393:VAL:HG12     | 2.30                     | 0.67              |
| 5:P:458:GLU:OE1      | 5:P:462:ARG:NH2      | 2.26                     | 0.67              |
| 7:Q16:327:LEU:CD1    | 7:Q16:358:PHE:CE1    | 2.76                     | 0.67              |
| 10:C16:1271:PHE:HE2  | 10:C16:1284:ASP:CB   | 2.06                     | 0.67              |
| 10:C16:1488:ILE:HD11 | 10:C16:1528:LEU:HD23 | 1.76                     | 0.67              |
| 10:C24:168:ARG:NH1   | 10:C24:229:PRO:CA    | 2.58                     | 0.67              |
| 10:C24:792:PHE:HD1   | 10:C24:850:ARG:NH1   | 1.92                     | 0.67              |
| 10:C24:1453:ARG:NH1  | 24:D24:1150:GLY:HA3  | 2.08                     | 0.67              |
| 10:C24:1661:LEU:O    | 10:C24:1662:ASP:C    | 2.29                     | 0.67              |
| 14:W:516:GLN:C       | 14:W:604:PRO:C       | 2.62                     | 0.67              |
| 10:C:453:LEU:HB2     | 10:C:486:LEU:CD2     | 2.22                     | 0.67              |
| 10:C8:639:MET:CE     | 10:C8:643:LEU:CD1    | 2.72                     | 0.67              |
| 11:A32:468:VAL:C     | 11:A32:470:LEU:H     | 2.00                     | 0.67              |
| 18:B:686:LEU:HD11    | 18:B:790:ASP:CG      | 2.17                     | 0.67              |
| 18:B:1831:LEU:CD1    | 18:B:1902:THR:HG23   | 2.25                     | 0.67              |
| 21:H:215:ARG:O       | 21:H:218:ILE:HG22    | 1.95                     | 0.67              |
| 21:H16:228:LEU:HD21  | 23:J16:592:VAL:HG12  | 1.76                     | 0.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1290:HIS:HB2  | 10:C32:1334:MET:CE   | 2.25                     | 0.67              |
| 10:C32:1348:LEU:CD1  | 10:C32:1359:ILE:CG1  | 2.72                     | 0.67              |
| 1:R:1228:ALA:HB2     | 1:R:1263:MET:HE2     | 1.75                     | 0.67              |
| 2:M8:428:SER:HB3     | 8:L8:355:SER:OG      | 1.94                     | 0.67              |
| 1:R16:1124:TRP:HZ2   | 4:T16:669:PRO:HG3    | 1.52                     | 0.67              |
| 5:P:109:ILE:HD13     | 14:W:18:PRO:CB       | 2.24                     | 0.67              |
| 5:P:375:LYS:NZ       | 14:W:83:GLU:OE2      | 2.28                     | 0.67              |
| 5:P:504:GLN:NE2      | 6:O:22:ASP:OD2       | 2.27                     | 0.67              |
| 9:K:751:LEU:CD2      | 9:K:754:ARG:HD3      | 2.25                     | 0.67              |
| 9:K8:751:LEU:HD22    | 9:K8:754:ARG:HD3     | 1.76                     | 0.67              |
| 9:K8:1074:ARG:NH1    | 9:K8:1126:LEU:CD2    | 2.58                     | 0.67              |
| 10:C16:8:VAL:CG2     | 10:C16:129:ASP:O     | 2.43                     | 0.67              |
| 10:C16:1385:LEU:HD23 | 10:C16:1389:ILE:HD11 | 1.77                     | 0.67              |
| 10:C16:1548:ILE:HG13 | 24:D8:1407:PHE:CE2   | 2.30                     | 0.67              |
| 11:A24:468:VAL:HG23  | 24:D16:1100:GLN:OE1  | 1.95                     | 0.67              |
| 10:C24:847:ARG:CZ    | 10:C24:911:ILE:N     | 2.57                     | 0.67              |
| 10:C24:1624:LEU:HD21 | 10:C24:1632:LEU:HD11 | 1.77                     | 0.67              |
| 10:C:168:ARG:NH1     | 10:C:229:PRO:CA      | 2.58                     | 0.67              |
| 10:C:1348:LEU:CD1    | 10:C:1359:ILE:CG1    | 2.72                     | 0.67              |
| 10:C8:345:MET:HE1    | 10:C8:401:ILE:HD13   | 1.40                     | 0.67              |
| 11:A16:676:TYR:HE2   | 24:D16:1395:SER:CA   | 2.05                     | 0.67              |
| 18:B8:152:HIS:CB     | 18:B8:163:ILE:HD13   | 2.24                     | 0.67              |
| 18:B8:313:ILE:HD12   | 18:B8:331:TRP:CE2    | 2.30                     | 0.67              |
| 21:H24:215:ARG:O     | 21:H24:218:ILE:HG22  | 1.95                     | 0.67              |
| 24:D:1099:ARG:CD     | 24:D:1149:VAL:HG11   | 2.21                     | 0.67              |
| 10:C32:647:GLU:OE1   | 10:C32:655:SER:HB3   | 1.95                     | 0.67              |
| 10:C32:1265:ARG:C    | 10:C32:1268:ARG:HE   | 2.02                     | 0.67              |
| 12:A48:198:PRO:HB2   | 12:A48:200:HIS:ND1   | 2.09                     | 0.67              |
| 2:M:625:HIS:CD2      | 3:N:225:PRO:HB3      | 2.30                     | 0.67              |
| 1:R8:1059:ILE:CB     | 24:D40:1435:ARG:NH2  | 2.58                     | 0.67              |
| 3:N8:200:MET:CE      | 3:N8:203:PHE:HD2     | 2.08                     | 0.67              |
| 2:M16:672:TYR:HB2    | 2:M16:680:LYS:HD3    | 1.73                     | 0.67              |
| 5:P:19:LYS:O         | 5:P:21:LYS:N         | 2.28                     | 0.67              |
| 5:P:55:ARG:HH12      | 5:P:64:ASP:CB        | 1.97                     | 0.67              |
| 5:P:500:ARG:HD2      | 6:O:290:MET:SD       | 2.35                     | 0.67              |
| 7:Q:30:ALA:CB        | 10:C8:815:GLN:HE22   | 2.08                     | 0.67              |
| 7:Q8:327:LEU:CD1     | 7:Q8:358:PHE:CE1     | 2.76                     | 0.67              |
| 5:P16:19:LYS:O       | 5:P16:21:LYS:N       | 2.28                     | 0.67              |
| 9:K8:1153:ALA:C      | 9:K8:1220:ASN:HD21   | 2.03                     | 0.67              |
| 10:C16:508:ILE:HG23  | 10:C16:549:TYR:OH    | 1.95                     | 0.67              |
| 11:A24:440:LEU:HD12  | 11:A24:443:LEU:HD11  | 1.75                     | 0.67              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:8:VAL:CG2     | 10:C24:129:ASP:O     | 2.43                     | 0.67              |
| 10:C24:1010:ALA:N    | 10:C24:1192:ARG:HH21 | 1.81                     | 0.67              |
| 10:C24:1507:LEU:C    | 10:C24:1509:SER:H    | 2.02                     | 0.67              |
| 11:A40:736:PRO:HB2   | 24:D32:871:ARG:NH1   | 2.10                     | 0.67              |
| 12:A:153:ARG:HG2     | 10:C8:74:ASP:CG      | 2.17                     | 0.67              |
| 12:A:198:PRO:HB2     | 12:A:200:HIS:ND1     | 2.09                     | 0.67              |
| 12:A:270:VAL:CG1     | 12:A:274:MET:HB3     | 2.25                     | 0.67              |
| 14:W:656:GLN:NE2     | 15:J:579:ARG:HB2     | 2.10                     | 0.67              |
| 10:C:1624:LEU:HD21   | 10:C:1632:LEU:HD11   | 1.77                     | 0.67              |
| 10:C8:453:LEU:HB2    | 10:C8:486:LEU:CD2    | 2.22                     | 0.67              |
| 10:C8:639:MET:HE3    | 10:C8:643:LEU:HD13   | 1.75                     | 0.67              |
| 10:C8:1271:PHE:CZ    | 10:C8:1284:ASP:CB    | 2.73                     | 0.67              |
| 10:C8:1385:LEU:HD23  | 10:C8:1389:ILE:HD11  | 1.77                     | 0.67              |
| 11:A16:91:GLU:CB     | 18:B:1112:LYS:HZ1    | 2.05                     | 0.67              |
| 11:A16:440:LEU:HD12  | 11:A16:443:LEU:HD11  | 1.75                     | 0.67              |
| 18:B:728:GLY:O       | 18:B:1197:VAL:HG23   | 1.95                     | 0.67              |
| 18:B:1911:LEU:HD13   | 18:B:1960:LEU:HD12   | 1.77                     | 0.67              |
| 18:B8:1390:LEU:CD1   | 18:B8:1404:LEU:HD11  | 2.25                     | 0.67              |
| 18:B8:1831:LEU:CD1   | 18:B8:1902:THR:HG23  | 2.25                     | 0.67              |
| 19:48:153:ARG:CZ     | 20:E8:467:ILE:HD11   | 2.24                     | 0.67              |
| 20:E8:341:TYR:O      | 20:E8:342:GLN:C      | 2.27                     | 0.67              |
| 10:C32:8:VAL:CG2     | 10:C32:129:ASP:O     | 2.43                     | 0.67              |
| 2:M:162:ILE:HD11     | 2:M:213:LEU:CD1      | 2.24                     | 0.66              |
| 1:R8:1466:LYS:CD     | 6:O8:160:LEU:HB2     | 2.21                     | 0.66              |
| 2:M8:278:VAL:CG1     | 2:M8:326:GLN:HG3     | 2.25                     | 0.66              |
| 2:M8:625:HIS:CD2     | 3:N8:225:PRO:HB3     | 2.30                     | 0.66              |
| 1:R16:1346:ILE:HD11  | 5:P16:685:PRO:CG     | 2.26                     | 0.66              |
| 9:K:1019:ARG:CZ      | 9:K:1059:ARG:HD3     | 2.25                     | 0.66              |
| 9:K:1248:LEU:CD1     | 9:K:1265:ILE:HD11    | 2.07                     | 0.66              |
| 9:K8:1085:TYR:CE1    | 9:K8:1093:SER:C      | 2.70                     | 0.66              |
| 10:C16:1624:LEU:HD21 | 10:C16:1632:LEU:HD11 | 1.77                     | 0.66              |
| 10:C16:1814:LYS:CE   | 23:J32:738:MET:SD    | 2.83                     | 0.66              |
| 10:C24:1333:HIS:CE1  | 10:C24:1337:LEU:CD2  | 2.77                     | 0.66              |
| 10:C24:1453:ARG:NH2  | 24:D24:1150:GLY:HA2  | 1.88                     | 0.66              |
| 11:A40:156:MET:CB    | 11:A40:555:HIS:CD2   | 2.47                     | 0.66              |
| 11:A40:270:VAL:CG1   | 11:A40:274:MET:HB3   | 2.25                     | 0.66              |
| 10:C:1290:HIS:HB2    | 10:C:1334:MET:CE     | 2.25                     | 0.66              |
| 10:C8:8:VAL:CG2      | 10:C8:129:ASP:O      | 2.43                     | 0.66              |
| 10:C8:57:VAL:HA      | 10:C8:62:ILE:HD11    | 1.77                     | 0.66              |
| 10:C8:647:GLU:OE1    | 10:C8:655:SER:HB3    | 1.95                     | 0.66              |
| 11:A32:72:ILE:CD1    | 21:H24:348:ALA:HA    | 2.24                     | 0.66              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:671:MET:HE3    | 18:B:736:ALA:HB3    | 1.76                     | 0.66              |
| 18:B8:729:LEU:CB    | 18:B8:1196:MET:HE1  | 2.23                     | 0.66              |
| 18:B8:1768:ILE:HD13 | 18:B8:1895:LEU:HD22 | 1.76                     | 0.66              |
| 18:B8:1945:TYR:CE2  | 18:B8:1946:LEU:HG   | 2.31                     | 0.66              |
| 18:B8:1947:GLU:HB3  | 18:B8:1948:PRO:HD3  | 1.76                     | 0.66              |
| 19:48:94:VAL:HA     | 19:48:97:LEU:HD12   | 1.77                     | 0.66              |
| 20:E8:235:HIS:NE2   | 20:E8:239:LYS:CE    | 2.55                     | 0.66              |
| 10:C32:798:VAL:HG12 | 10:C32:802:TRP:CE2  | 2.29                     | 0.66              |
| 1:R:1168:LEU:HD23   | 1:R:1216:ILE:CG1    | 2.24                     | 0.66              |
| 1:R8:1466:LYS:HD2   | 6:O8:160:LEU:CG     | 2.24                     | 0.66              |
| 2:M8:571:TYR:CD1    | 2:M8:595:LEU:CD1    | 2.77                     | 0.66              |
| 2:M16:278:VAL:CG1   | 2:M16:326:GLN:HG3   | 2.25                     | 0.66              |
| 5:P8:207:HIS:CD2    | 5:P8:393:VAL:HG12   | 2.30                     | 0.66              |
| 5:P16:187:TRP:CZ3   | 5:P16:191:ARG:HG2   | 2.30                     | 0.66              |
| 9:K:614:PHE:CA      | 9:K:683:GLN:NE2     | 2.58                     | 0.66              |
| 9:K8:1071:PHE:CZ    | 9:K8:1107:LEU:HD23  | 2.30                     | 0.66              |
| 10:C16:1333:HIS:CE1 | 10:C16:1337:LEU:CD2 | 2.78                     | 0.66              |
| 10:C16:1507:LEU:C   | 10:C16:1509:SER:H   | 2.02                     | 0.66              |
| 10:C24:453:LEU:HB2  | 10:C24:486:LEU:CD2  | 2.23                     | 0.66              |
| 10:C24:1708:ARG:NH2 | 21:H24:275:LYS:CE   | 2.56                     | 0.66              |
| 14:W:715:ASP:CG     | 10:C8:1568:ARG:HD3  | 2.19                     | 0.66              |
| 10:C:647:GLU:OE1    | 10:C:655:SER:HB3    | 1.95                     | 0.66              |
| 10:C:1488:ILE:CD1   | 10:C:1528:LEU:HD23  | 2.26                     | 0.66              |
| 10:C8:768:ARG:CZ    | 10:C8:775:LYS:CG    | 2.69                     | 0.66              |
| 11:A32:845:THR:OG1  | 24:D32:1297:HIS:CE1 | 2.48                     | 0.66              |
| 18:B:410:GLN:CG     | 18:B:538:ARG:HH22   | 2.08                     | 0.66              |
| 18:B:729:LEU:CB     | 18:B:1196:MET:HE1   | 2.23                     | 0.66              |
| 18:B:1768:ILE:HD13  | 18:B:1895:LEU:HD22  | 1.76                     | 0.66              |
| 18:B:1768:ILE:HD13  | 18:B:1895:LEU:CD2   | 2.24                     | 0.66              |
| 18:B:1945:TYR:CE2   | 18:B:1946:LEU:HG    | 2.31                     | 0.66              |
| 18:B8:286:GLN:OE1   | 18:B8:443:PHE:CG    | 2.49                     | 0.66              |
| 18:B8:638:ALA:HA    | 18:B8:699:MET:HE3   | 1.76                     | 0.66              |
| 19:4:15:ILE:HD12    | 19:4:20:ILE:HD11    | 1.77                     | 0.66              |
| 19:4:186:GLY:C      | 19:4:187:SER:O      | 2.38                     | 0.66              |
| 21:H8:228:LEU:HD21  | 23:J8:592:VAL:HG12  | 1.77                     | 0.66              |
| 12:A48:259:ILE:HG22 | 12:A48:276:LEU:HD22 | 1.75                     | 0.66              |
| 12:A48:270:VAL:CG1  | 12:A48:274:MET:HB3  | 2.25                     | 0.66              |
| 12:A48:374:PHE:HE2  | 12:A48:426:ILE:HD12 | 1.61                     | 0.66              |
| 1:R8:1265:PHE:CD2   | 1:R8:1269:LEU:CD1   | 2.77                     | 0.66              |
| 2:M8:257:VAL:HG23   | 2:M8:274:VAL:HG21   | 1.78                     | 0.66              |
| 2:M8:363:ARG:HH12   | 2:M8:494:SER:HB2    | 1.59                     | 0.66              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P8:19:LYS:O        | 5:P8:21:LYS:N        | 2.28                     | 0.66              |
| 6:O16:119:ARG:HH22   | 6:O16:182:GLU:HG2    | 1.59                     | 0.66              |
| 9:K8:578:THR:CG2     | 9:K8:616:ARG:HH21    | 1.85                     | 0.66              |
| 11:A24:307:GLY:HA3   | 20:E:387:LEU:CD2     | 2.26                     | 0.66              |
| 13:V:844:MET:CG      | 10:C8:1502:ARG:HH21  | 1.73                     | 0.66              |
| 10:C:1234:ASP:OD1    | 10:C:1302:LYS:NZ     | 2.25                     | 0.66              |
| 10:C:1358:ASP:C      | 10:C:1360:GLN:N      | 2.53                     | 0.66              |
| 10:C:1661:LEU:O      | 10:C:1662:ASP:C      | 2.29                     | 0.66              |
| 11:A16:56:ALA:C      | 11:A16:58:SER:N      | 2.49                     | 0.66              |
| 18:B:241:TYR:CE1     | 18:B:245:LEU:HD11    | 2.30                     | 0.66              |
| 18:B:1618:HIS:ND1    | 18:B:1622:ILE:HD11   | 2.09                     | 0.66              |
| 22:I8:199:PHE:CD1    | 23:J8:620:MET:CG     | 2.76                     | 0.66              |
| 21:H16:207:GLN:NE2   | 23:J16:572:ASP:OD1   | 2.26                     | 0.66              |
| 21:H16:215:ARG:O     | 21:H16:218:ILE:HG22  | 1.95                     | 0.66              |
| 10:C32:1488:ILE:HD11 | 10:C32:1528:LEU:HD23 | 1.76                     | 0.66              |
| 1:R8:1185:THR:HG21   | 24:D40:1462:PHE:CE2  | 2.26                     | 0.66              |
| 1:R8:1466:LYS:HB3    | 6:O8:160:LEU:HD11    | 1.74                     | 0.66              |
| 2:M8:503:TYR:CE1     | 2:M8:507:LEU:CD1     | 2.79                     | 0.66              |
| 1:R16:1340:LEU:HD23  | 1:R16:1374:MET:SD    | 2.35                     | 0.66              |
| 4:T8:671:ILE:HD11    | 5:P8:698:GLY:HA3     | 1.78                     | 0.66              |
| 5:P:401:ARG:CB       | 5:P:414:VAL:HG11     | 2.25                     | 0.66              |
| 5:P:578:LEU:HD13     | 5:P:608:LYS:NZ       | 2.11                     | 0.66              |
| 9:K:577:GLN:NE2      | 9:K:625:ARG:HH11     | 1.93                     | 0.66              |
| 9:K:1019:ARG:HD3     | 9:K:1059:ARG:HD2     | 1.75                     | 0.66              |
| 9:K:1153:ALA:C       | 9:K:1220:ASN:HD21    | 2.03                     | 0.66              |
| 9:K8:614:PHE:HA      | 9:K8:683:GLN:NE2     | 2.11                     | 0.66              |
| 10:C24:508:ILE:HG23  | 10:C24:549:TYR:OH    | 1.95                     | 0.66              |
| 10:C24:557:VAL:HG22  | 10:C24:565:ARG:CZ    | 2.26                     | 0.66              |
| 10:C24:1290:HIS:HB2  | 10:C24:1334:MET:CE   | 2.25                     | 0.66              |
| 10:C24:1385:LEU:HD23 | 10:C24:1389:ILE:HD11 | 1.77                     | 0.66              |
| 11:A40:326:TYR:OH    | 17:F16:74:ILE:O      | 2.12                     | 0.66              |
| 11:A40:707:LEU:HD21  | 11:A40:767:ARG:HH22  | 1.59                     | 0.66              |
| 14:W:676:PHE:CE1     | 14:W:680:ARG:HD2     | 2.31                     | 0.66              |
| 10:C:278:ARG:HH11    | 10:C:287:SER:HB2     | 1.56                     | 0.66              |
| 10:C:847:ARG:HD2     | 10:C:911:ILE:HD12    | 1.77                     | 0.66              |
| 10:C8:1488:ILE:CD1   | 10:C8:1528:LEU:HD23  | 2.26                     | 0.66              |
| 18:B:457:SER:CA      | 18:B:548:ARG:NH1     | 2.50                     | 0.66              |
| 18:B8:241:TYR:CE1    | 18:B8:245:LEU:HD11   | 2.30                     | 0.66              |
| 24:D40:865:VAL:CG2   | 24:D40:928:THR:HG21  | 2.25                     | 0.66              |
| 10:C32:398:SER:HA    | 10:C32:458:VAL:HG11  | 1.78                     | 0.66              |
| 10:C32:513:LEU:HD13  | 10:C32:549:TYR:HB3   | 1.76                     | 0.66              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C32:1251:PHE:HZ  | 10:C32:1319:ARG:CZ   | 1.99                     | 0.66              |
| 10:C32:1358:ASP:C   | 10:C32:1360:GLN:N    | 2.53                     | 0.66              |
| 1:R8:1340:LEU:HD23  | 1:R8:1374:MET:SD     | 2.35                     | 0.66              |
| 1:R8:1449:TRP:HH2   | 2:M8:161:ASP:O       | 1.76                     | 0.66              |
| 3:N16:200:MET:CE    | 3:N16:203:PHE:HD2    | 2.08                     | 0.66              |
| 10:C16:513:LEU:HD13 | 10:C16:549:TYR:HB3   | 1.76                     | 0.66              |
| 10:C24:386:ASN:HB3  | 10:C24:449:GLU:OE1   | 1.94                     | 0.66              |
| 10:C24:1488:ILE:CD1 | 10:C24:1528:LEU:HD23 | 2.26                     | 0.66              |
| 11:A40:374:PHE:HE2  | 11:A40:426:ILE:HD12  | 1.60                     | 0.66              |
| 13:V:832:LEU:HD23   | 13:V:836:LEU:CB      | 2.25                     | 0.66              |
| 10:C:1002:LEU:HD12  | 10:C:1019:ARG:HH12   | 1.61                     | 0.66              |
| 10:C8:1824:ARG:O    | 10:C8:1828:THR:OG1   | 2.13                     | 0.66              |
| 11:A16:270:VAL:CG1  | 11:A16:274:MET:HB3   | 2.25                     | 0.66              |
| 11:A16:703:ALA:CA   | 24:D16:1398:ARG:HD3  | 2.20                     | 0.66              |
| 11:A32:714:GLY:HA2  | 24:D32:1398:ARG:CZ   | 2.25                     | 0.66              |
| 11:A32:841:LEU:CD1  | 11:A32:857:VAL:HG21  | 2.26                     | 0.66              |
| 18:B:313:ILE:HD12   | 18:B:331:TRP:CE2     | 2.30                     | 0.66              |
| 18:B:1112:LYS:HE2   | 21:H:327:SER:HB3     | 1.76                     | 0.66              |
| 18:B8:171:ILE:HD13  | 18:B8:226:TYR:CB     | 2.25                     | 0.66              |
| 18:B8:410:GLN:CG    | 18:B8:538:ARG:HH22   | 2.08                     | 0.66              |
| 18:B8:1161:LEU:CD1  | 18:B8:1403:ILE:HD13  | 2.26                     | 0.66              |
| 21:H8:316:ILE:O     | 21:H8:317:ALA:C      | 2.35                     | 0.66              |
| 22:I24:199:PHE:CE1  | 23:J24:620:MET:HG3   | 2.31                     | 0.66              |
| 1:R:1340:LEU:HD23   | 1:R:1374:MET:SD      | 2.35                     | 0.66              |
| 6:O8:119:ARG:HH21   | 6:O8:182:GLU:CB      | 2.08                     | 0.66              |
| 5:P16:281:ILE:HD11  | 5:P16:341:MET:HE2    | 1.78                     | 0.66              |
| 5:P16:500:ARG:HD2   | 6:O16:290:MET:SD     | 2.35                     | 0.66              |
| 5:P16:578:LEU:HD13  | 5:P16:608:LYS:NZ     | 2.10                     | 0.66              |
| 8:L8:605:MET:SD     | 8:L8:631:LEU:HD13    | 2.35                     | 0.66              |
| 10:C16:1688:ARG:HG3 | 23:J32:735:LYS:NZ    | 2.09                     | 0.66              |
| 10:C24:647:GLU:OE2  | 10:C24:656:THR:OG1   | 2.13                     | 0.66              |
| 10:C24:1688:ARG:CG  | 23:J24:735:LYS:CE    | 2.56                     | 0.66              |
| 11:A40:468:VAL:HG21 | 24:D32:1100:GLN:CG   | 2.23                     | 0.66              |
| 14:W:586:ILE:HG12   | 15:J:572:ASP:OD2     | 1.96                     | 0.66              |
| 10:C:647:GLU:OE2    | 10:C:656:THR:OG1     | 2.13                     | 0.66              |
| 10:C:1271:PHE:HE2   | 10:C:1284:ASP:CB     | 2.06                     | 0.66              |
| 10:C8:565:ARG:HD3   | 10:C8:568:TRP:CD2    | 2.17                     | 0.66              |
| 10:C8:1290:HIS:HB2  | 10:C8:1334:MET:CE    | 2.25                     | 0.66              |
| 10:C8:1488:ILE:HD11 | 10:C8:1528:LEU:HD23  | 1.76                     | 0.66              |
| 11:A16:52:LEU:CD2   | 11:A16:55:GLU:OE2    | 2.37                     | 0.66              |
| 11:A16:841:LEU:CD1  | 11:A16:857:VAL:HG21  | 2.26                     | 0.66              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A32:326:TYR:OH    | 17:F24:74:ILE:O     | 2.12                     | 0.66              |
| 11:A32:342:VAL:CG1   | 17:F24:77:TYR:CE1   | 2.78                     | 0.66              |
| 18:B:904:ALA:CB      | 18:B:917:PHE:HZ     | 2.08                     | 0.66              |
| 18:B:1148:ILE:HG12   | 18:B:1371:VAL:CG2   | 2.26                     | 0.66              |
| 18:B:1161:LEU:CD1    | 18:B:1403:ILE:HD13  | 2.26                     | 0.66              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:HD12  | 1.77                     | 0.66              |
| 18:B8:690:TRP:CH2    | 18:B8:787:VAL:HG22  | 2.26                     | 0.66              |
| 18:B8:1148:ILE:HG12  | 18:B8:1371:VAL:CG2  | 2.26                     | 0.66              |
| 10:C32:169:GLN:OE1   | 10:C32:169:GLN:CA   | 2.44                     | 0.66              |
| 10:C32:1274:ALA:C    | 10:C32:1276:SER:N   | 2.48                     | 0.66              |
| 3:N:162:THR:HG22     | 3:N:168:VAL:CG2     | 2.16                     | 0.66              |
| 2:M16:627:TYR:OH     | 3:N16:163:ALA:O     | 2.13                     | 0.66              |
| 7:Q8:143:ARG:CZ      | 7:Q8:147:GLU:OE2    | 2.44                     | 0.66              |
| 7:Q16:143:ARG:CZ     | 7:Q16:147:GLU:OE2   | 2.44                     | 0.66              |
| 9:K8:1074:ARG:CD     | 9:K8:1126:LEU:CD2   | 2.71                     | 0.66              |
| 10:C24:1593:TRP:CZ2  | 10:C24:1603:PHE:CD2 | 2.82                     | 0.66              |
| 11:A40:103:GLU:HG2   | 21:H16:323:TYR:HE2  | 1.61                     | 0.66              |
| 13:V:861:PHE:HB3     | 14:W:741:ARG:CZ     | 2.25                     | 0.66              |
| 15:J:576:LEU:HD23    | 15:J:576:LEU:C      | 2.21                     | 0.66              |
| 10:C8:1129:VAL:HG12  | 10:C8:1130:SER:N    | 2.11                     | 0.66              |
| 10:C8:1593:TRP:CZ2   | 10:C8:1603:PHE:CD2  | 2.82                     | 0.66              |
| 11:A16:496:LYS:NZ    | 17:F8:64:ASP:OD2    | 2.27                     | 0.66              |
| 18:B:195:MET:SD      | 18:B:199:LEU:HD23   | 2.36                     | 0.66              |
| 18:B:1342:LEU:CD2    | 18:B:1406:ALA:CB    | 2.69                     | 0.66              |
| 22:I:199:PHE:CD1     | 23:J32:620:MET:CG   | 2.76                     | 0.66              |
| 24:D:275:LYS:HE3     | 24:D:294:GLU:CD     | 2.21                     | 0.66              |
| 24:D8:275:LYS:HE3    | 24:D8:294:GLU:CD    | 2.21                     | 0.66              |
| 24:D32:275:LYS:HE3   | 24:D32:294:GLU:CD   | 2.21                     | 0.66              |
| 24:D32:280:VAL:HG21  | 24:D32:373:PRO:HG2  | 1.78                     | 0.66              |
| 10:C32:225:LEU:HD22  | 10:C32:388:TYR:OH   | 1.96                     | 0.66              |
| 1:R:1165:MET:HE1     | 1:R:1220:GLN:HG2    | 1.76                     | 0.66              |
| 2:M:503:TYR:CE1      | 2:M:507:LEU:CD1     | 2.79                     | 0.66              |
| 5:P8:175:MET:SD      | 5:P8:433:LEU:CD2    | 2.84                     | 0.66              |
| 5:P8:611:LEU:CG      | 5:P8:629:ARG:HD3    | 2.20                     | 0.66              |
| 5:P16:207:HIS:CD2    | 5:P16:393:VAL:HG12  | 2.30                     | 0.66              |
| 11:A24:270:VAL:CG1   | 11:A24:274:MET:HB3  | 2.25                     | 0.66              |
| 10:C24:1129:VAL:HG12 | 10:C24:1130:SER:N   | 2.11                     | 0.66              |
| 10:C24:1271:PHE:HE2  | 10:C24:1284:ASP:CB  | 2.06                     | 0.66              |
| 10:C24:1824:ARG:O    | 10:C24:1828:THR:OG1 | 2.13                     | 0.66              |
| 11:A40:496:LYS:NZ    | 17:F16:64:ASP:OD2   | 2.26                     | 0.66              |
| 11:A40:842:ALA:O     | 11:A40:845:THR:HG23 | 1.96                     | 0.66              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 14:W:806:GLU:CD     | 15:J:716:ARG:HH21    | 2.03                     | 0.66              |
| 15:J:680:LEU:HD23   | 15:J:686:MET:HE3     | 1.77                     | 0.66              |
| 10:C:228:ARG:HH22   | 10:C:277:SER:HB3     | 1.57                     | 0.66              |
| 10:C:847:ARG:CZ     | 10:C:911:ILE:N       | 2.57                     | 0.66              |
| 10:C:1333:HIS:CE1   | 10:C:1337:LEU:CD2    | 2.78                     | 0.66              |
| 10:C8:508:ILE:HG23  | 10:C8:549:TYR:OH     | 1.95                     | 0.66              |
| 10:C8:1621:LYS:O    | 10:C8:1622:SER:C     | 2.35                     | 0.66              |
| 11:A16:676:TYR:OH   | 24:D16:1394:SER:O    | 2.14                     | 0.66              |
| 18:B8:177:ARG:HG3   | 18:B8:233:ARG:HH21   | 1.61                     | 0.66              |
| 18:B8:1291:LEU:HD11 | 18:B8:1332:VAL:CG2   | 2.25                     | 0.66              |
| 18:B8:1900:ILE:HD12 | 18:B8:1946:LEU:CD2   | 2.26                     | 0.66              |
| 19:4:94:VAL:HA      | 19:4:97:LEU:HD12     | 1.77                     | 0.66              |
| 21:H:207:GLN:NE2    | 23:J32:572:ASP:OD1   | 2.26                     | 0.66              |
| 22:I16:300:LEU:CD1  | 23:J16:689:LEU:CD2   | 2.73                     | 0.66              |
| 24:D24:280:VAL:HG21 | 24:D24:373:PRO:HG2   | 1.78                     | 0.66              |
| 10:C32:1777:SER:O   | 10:C32:1778:ASN:C    | 2.26                     | 0.66              |
| 2:M:278:VAL:CG1     | 2:M:326:GLN:HG3      | 2.25                     | 0.66              |
| 2:M:367:SER:HB2     | 2:M:486:MET:HE1      | 1.78                     | 0.66              |
| 3:N:200:MET:CE      | 3:N:203:PHE:HD2      | 2.08                     | 0.66              |
| 1:R8:1466:LYS:CG    | 6:O8:160:LEU:HD13    | 2.26                     | 0.66              |
| 5:P8:55:ARG:HH12    | 5:P8:64:ASP:CB       | 1.97                     | 0.66              |
| 5:P8:105:ARG:CZ     | 5:P8:130:VAL:CG2     | 2.72                     | 0.66              |
| 5:P8:500:ARG:HD2    | 6:O8:290:MET:SD      | 2.35                     | 0.66              |
| 9:K8:645:GLU:O      | 9:K8:649:MET:HG3     | 1.96                     | 0.66              |
| 9:K8:923:ILE:HG22   | 9:K8:929:ARG:NE      | 2.10                     | 0.66              |
| 10:C16:57:VAL:HA    | 10:C16:62:ILE:HD11   | 1.76                     | 0.66              |
| 10:C16:1488:ILE:CD1 | 10:C16:1528:LEU:HD23 | 2.26                     | 0.66              |
| 10:C16:1593:TRP:CZ2 | 10:C16:1603:PHE:CD2  | 2.82                     | 0.66              |
| 11:A40:342:VAL:CG1  | 17:F16:77:TYR:CE1    | 2.78                     | 0.66              |
| 14:W:518:GLU:N      | 14:W:605:ASN:ND2     | 2.43                     | 0.66              |
| 10:C:1488:ILE:HD11  | 10:C:1528:LEU:HD23   | 1.76                     | 0.66              |
| 11:A32:159:LYS:HZ2  | 18:B8:1918:ARG:HG3   | 1.61                     | 0.66              |
| 11:A32:711:ARG:HD3  | 24:D32:1398:ARG:HG2  | 1.75                     | 0.66              |
| 18:B8:1736:ALA:HB3  | 18:B8:1871:GLN:NE2   | 2.10                     | 0.66              |
| 19:48:15:ILE:HD12   | 19:48:20:ILE:HD11    | 1.77                     | 0.66              |
| 19:48:186:GLY:C     | 19:48:187:SER:O      | 2.38                     | 0.66              |
| 22:I8:300:LEU:CD1   | 23:J8:689:LEU:CD2    | 2.73                     | 0.66              |
| 21:H16:316:ILE:O    | 21:H16:317:ALA:C     | 2.35                     | 0.66              |
| 22:I16:199:PHE:CD1  | 23:J16:620:MET:CG    | 2.76                     | 0.66              |
| 10:C32:182:ASP:HB2  | 10:C32:183:PRO:CD    | 2.23                     | 0.66              |
| 10:C32:453:LEU:CD2  | 10:C32:459:LEU:CD1   | 2.66                     | 0.66              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 12:A48:841:LEU:CD1   | 12:A48:857:VAL:HG21 | 2.26                     | 0.66              |
| 1:R:1139:ARG:HG3     | 1:R:1157:ARG:NH1    | 2.11                     | 0.66              |
| 2:M:348:GLU:O        | 2:M:350:SER:N       | 2.29                     | 0.66              |
| 2:M:377:ARG:HH12     | 2:M:477:ASP:HB2     | 1.61                     | 0.66              |
| 3:N:267:TRP:HH2      | 3:N:294:TRP:HH2     | 1.43                     | 0.66              |
| 2:M8:162:ILE:HD11    | 2:M8:213:LEU:CD1    | 2.24                     | 0.66              |
| 2:M16:363:ARG:HH12   | 2:M16:494:SER:HB2   | 1.59                     | 0.66              |
| 2:M16:627:TYR:OH     | 3:N16:162:THR:HB    | 1.96                     | 0.66              |
| 9:K:1074:ARG:NH1     | 9:K:1126:LEU:CD2    | 2.58                     | 0.66              |
| 10:C16:878:ARG:HH21  | 10:C16:885:VAL:CG2  | 2.09                     | 0.66              |
| 10:C24:225:LEU:HD22  | 10:C24:388:TYR:OH   | 1.96                     | 0.66              |
| 10:C24:1133:ILE:HG12 | 10:C24:1152:LYS:HD2 | 1.78                     | 0.66              |
| 11:A40:841:LEU:CD1   | 11:A40:857:VAL:HG21 | 2.26                     | 0.66              |
| 11:A16:842:ALA:O     | 11:A16:845:THR:HG23 | 1.96                     | 0.66              |
| 18:B:152:HIS:CB      | 18:B:163:ILE:HD13   | 2.24                     | 0.66              |
| 18:B:684:ILE:HD11    | 24:D16:1065:ALA:CB  | 2.26                     | 0.66              |
| 18:B:1291:LEU:HD11   | 18:B:1332:VAL:CG2   | 2.25                     | 0.66              |
| 18:B:1736:ALA:HB3    | 18:B:1871:GLN:NE2   | 2.10                     | 0.66              |
| 18:B8:241:TYR:CB     | 18:B8:271:LEU:HD23  | 2.26                     | 0.66              |
| 18:B8:1657:TYR:CE2   | 18:B8:1658:MET:HG2  | 2.31                     | 0.66              |
| 19:4:153:ARG:HH21    | 20:E:467:ILE:CD1    | 2.00                     | 0.66              |
| 21:H24:207:GLN:NE2   | 23:J24:572:ASP:OD1  | 2.26                     | 0.66              |
| 24:D8:94:ALA:CB      | 24:D8:543:MET:HE1   | 2.26                     | 0.66              |
| 24:D8:1452:LYS:NZ    | 24:D16:971:HIS:CE1  | 2.63                     | 0.66              |
| 24:D40:275:LYS:HE3   | 24:D40:294:GLU:CD   | 2.21                     | 0.66              |
| 24:D40:839:GLU:O     | 24:D40:971:HIS:CE1  | 2.48                     | 0.66              |
| 2:M:448:ASP:OD1      | 2:M:448:ASP:N       | 2.21                     | 0.65              |
| 3:N8:15:HIS:HE2      | 3:N8:31:SER:HG      | 1.42                     | 0.65              |
| 5:P8:105:ARG:HH12    | 5:P8:130:VAL:HG13   | 1.59                     | 0.65              |
| 8:L16:1026:ARG:HB3   | 9:K16:1284:MET:HG2  | 1.77                     | 0.65              |
| 10:C16:169:GLN:OE1   | 10:C16:169:GLN:CA   | 2.44                     | 0.65              |
| 10:C16:1348:LEU:CD1  | 10:C16:1359:ILE:CG1 | 2.72                     | 0.65              |
| 11:A24:841:LEU:CD1   | 11:A24:857:VAL:HG21 | 2.26                     | 0.65              |
| 10:C24:390:HIS:HB3   | 10:C24:452:LEU:CB   | 2.22                     | 0.65              |
| 10:C24:1348:LEU:CD1  | 10:C24:1359:ILE:CG1 | 2.72                     | 0.65              |
| 11:A40:390:ALA:HB2   | 24:D32:1099:ARG:HB2 | 1.77                     | 0.65              |
| 11:A40:743:ARG:NH2   | 24:D32:699:HIS:CE1  | 2.53                     | 0.65              |
| 14:W:265:MET:HE2     | 14:W:301:LEU:HD23   | 1.76                     | 0.65              |
| 10:C:153:ALA:CB      | 24:D:1403:LEU:HD11  | 2.12                     | 0.65              |
| 10:C:508:ILE:HG23    | 10:C:549:TYR:OH     | 1.94                     | 0.65              |
| 10:C:878:ARG:HH21    | 10:C:885:VAL:CG2    | 2.09                     | 0.65              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:1297:HIS:NE2    | 10:C:1372:ALA:HB1    | 2.11                     | 0.65              |
| 10:C8:300:VAL:HG12   | 10:C8:317:ARG:HG3    | 1.78                     | 0.65              |
| 10:C8:1358:ASP:C     | 10:C8:1360:GLN:N     | 2.53                     | 0.65              |
| 11:A32:842:ALA:O     | 11:A32:845:THR:HG23  | 1.96                     | 0.65              |
| 18:B:1110:LEU:HD12   | 21:H:323:TYR:HH      | 1.61                     | 0.65              |
| 18:B8:1156:GLN:C     | 18:B8:1382:LYS:HZ3   | 2.04                     | 0.65              |
| 19:4:295:SER:HB2     | 24:D24:224:ARG:NH2   | 2.11                     | 0.65              |
| 22:I24:300:LEU:CD1   | 23:J24:689:LEU:CD2   | 2.73                     | 0.65              |
| 24:D:387:LEU:O       | 24:D16:746:ALA:HB3   | 1.96                     | 0.65              |
| 24:D:409:LEU:HD22    | 24:D16:746:ALA:N     | 2.08                     | 0.65              |
| 24:D24:1428:ASN:CG   | 24:D32:968:ILE:HD11  | 2.22                     | 0.65              |
| 24:D40:873:ARG:HH11  | 24:D40:884:ASP:CG    | 2.04                     | 0.65              |
| 10:C32:620:PRO:HB3   | 10:C32:636:VAL:HG13  | 1.58                     | 0.65              |
| 12:A48:842:ALA:O     | 12:A48:845:THR:HG23  | 1.96                     | 0.65              |
| 9:K8:577:GLN:NE2     | 9:K8:625:ARG:HH11    | 1.93                     | 0.65              |
| 10:C16:390:HIS:HB3   | 10:C16:452:LEU:CB    | 2.23                     | 0.65              |
| 10:C16:717:GLU:O     | 10:C16:719:PRO:CD    | 2.44                     | 0.65              |
| 10:C16:1129:VAL:HG12 | 10:C16:1130:SER:N    | 2.11                     | 0.65              |
| 10:C24:717:GLU:O     | 10:C24:719:PRO:CD    | 2.44                     | 0.65              |
| 10:C24:1251:PHE:HZ   | 10:C24:1319:ARG:CZ   | 1.99                     | 0.65              |
| 11:A40:803:PRO:HB3   | 24:D24:1401:LEU:HD11 | 1.67                     | 0.65              |
| 14:W:711:ARG:NH1     | 10:C8:1606:GLY:CA    | 2.59                     | 0.65              |
| 10:C8:847:ARG:HD2    | 10:C8:911:ILE:HD12   | 1.77                     | 0.65              |
| 10:C8:1624:LEU:HD21  | 10:C8:1632:LEU:HD11  | 1.77                     | 0.65              |
| 22:I16:199:PHE:CE1   | 23:J16:620:MET:HG3   | 2.31                     | 0.65              |
| 10:C32:168:ARG:NH1   | 10:C32:229:PRO:CA    | 2.58                     | 0.65              |
| 10:C32:1163:LEU:CD2  | 10:C32:1166:SER:CB   | 2.74                     | 0.65              |
| 10:C32:1385:LEU:HD23 | 10:C32:1389:ILE:HD11 | 1.77                     | 0.65              |
| 2:M:257:VAL:HG23     | 2:M:274:VAL:HG21     | 1.78                     | 0.65              |
| 1:R16:1191:LYS:O     | 1:R16:1192:LYS:C     | 2.35                     | 0.65              |
| 5:P:303:LYS:HG3      | 5:P:373:PHE:CE1      | 2.31                     | 0.65              |
| 6:O:119:ARG:HH21     | 6:O:182:GLU:CB       | 2.08                     | 0.65              |
| 6:O16:179:LYS:C      | 6:O16:180:GLY:O      | 2.39                     | 0.65              |
| 8:L:346:TRP:CH2      | 8:L:350:THR:CG2      | 2.78                     | 0.65              |
| 8:L16:1081:MET:SD    | 9:K16:1083:ILE:HG22  | 2.36                     | 0.65              |
| 9:K:645:GLU:O        | 9:K:649:MET:HG3      | 1.96                     | 0.65              |
| 10:C16:390:HIS:CB    | 10:C16:452:LEU:HB2   | 2.24                     | 0.65              |
| 10:C16:1716:LYS:HG3  | 10:C16:1721:GLN:HE21 | 1.61                     | 0.65              |
| 10:C24:719:PRO:C     | 10:C24:721:PHE:H     | 2.05                     | 0.65              |
| 10:C24:1716:LYS:HG3  | 10:C24:1721:GLN:HE21 | 1.61                     | 0.65              |
| 12:A:643:SER:H       | 12:A:685:ARG:NH1     | 1.93                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:W:659:ARG:HB3    | 15:J:586:GLU:OE1    | 1.97                     | 0.65              |
| 10:C:8:VAL:CG2      | 10:C:129:ASP:O      | 2.43                     | 0.65              |
| 10:C:225:LEU:HD22   | 10:C:388:TYR:OH     | 1.96                     | 0.65              |
| 10:C:572:ILE:CG1    | 10:C:606:MET:HE1    | 2.26                     | 0.65              |
| 10:C:1129:VAL:HG12  | 10:C:1130:SER:N     | 2.11                     | 0.65              |
| 10:C:1424:GLN:HE21  | 10:C:1478:VAL:CG1   | 2.10                     | 0.65              |
| 10:C:1593:TRP:CZ2   | 10:C:1603:PHE:CD2   | 2.82                     | 0.65              |
| 11:A16:159:LYS:HZ2  | 18:B:1918:ARG:HG3   | 1.62                     | 0.65              |
| 18:B:86:LYS:CD      | 18:B:123:LEU:HD11   | 2.26                     | 0.65              |
| 18:B:241:TYR:CB     | 18:B:271:LEU:HD23   | 2.26                     | 0.65              |
| 18:B:676:ASP:O      | 18:B:678:PRO:CD     | 2.40                     | 0.65              |
| 18:B8:750:GLU:CG    | 18:B8:760:ARG:CZ    | 2.73                     | 0.65              |
| 20:E:202:ASP:C      | 20:E:204:SER:N      | 2.47                     | 0.65              |
| 22:I:300:LEU:CD1    | 23:J32:689:LEU:CD2  | 2.73                     | 0.65              |
| 21:H16:262:GLU:CD   | 23:J16:648:TYR:OH   | 2.39                     | 0.65              |
| 24:D:280:VAL:HG21   | 24:D:373:PRO:HG2    | 1.78                     | 0.65              |
| 24:D16:280:VAL:HG21 | 24:D16:373:PRO:HG2  | 1.78                     | 0.65              |
| 24:D32:94:ALA:CB    | 24:D32:543:MET:HE1  | 2.27                     | 0.65              |
| 10:C32:390:HIS:HB3  | 10:C32:452:LEU:CB   | 2.23                     | 0.65              |
| 2:M:342:VAL:CG1     | 2:M:343:MET:H       | 1.92                     | 0.65              |
| 2:M8:755:THR:HB     | 2:M8:757:VAL:HG23   | 1.79                     | 0.65              |
| 2:M16:310:HIS:HA    | 2:M16:313:MET:HE2   | 1.78                     | 0.65              |
| 5:P8:578:LEU:HD13   | 5:P8:608:LYS:NZ     | 2.11                     | 0.65              |
| 5:P16:614:VAL:HG11  | 5:P16:626:ALA:HB2   | 1.79                     | 0.65              |
| 9:K:751:LEU:HD22    | 9:K:754:ARG:NH1     | 2.12                     | 0.65              |
| 10:C16:1297:HIS:NE2 | 10:C16:1372:ALA:HB1 | 2.11                     | 0.65              |
| 11:A24:496:LYS:NZ   | 17:F:64:ASP:OD2     | 2.26                     | 0.65              |
| 11:A24:842:ALA:O    | 11:A24:845:THR:HG23 | 1.96                     | 0.65              |
| 12:A:841:LEU:CD1    | 12:A:857:VAL:HG21   | 2.26                     | 0.65              |
| 14:W:516:GLN:O      | 14:W:604:PRO:HB2    | 1.96                     | 0.65              |
| 10:C:1385:LEU:HD23  | 10:C:1389:ILE:HD11  | 1.77                     | 0.65              |
| 10:C8:225:LEU:HD22  | 10:C8:388:TYR:OH    | 1.96                     | 0.65              |
| 11:A16:342:VAL:CG1  | 17:F8:77:TYR:CE1    | 2.78                     | 0.65              |
| 11:A16:702:GLU:OE2  | 24:D16:1395:SER:OG  | 2.13                     | 0.65              |
| 18:B:1900:ILE:HD12  | 18:B:1946:LEU:CD2   | 2.26                     | 0.65              |
| 18:B:1947:GLU:HB3   | 18:B:1948:PRO:HD3   | 1.76                     | 0.65              |
| 18:B8:344:LYS:HE3   | 18:B8:350:LEU:O     | 1.96                     | 0.65              |
| 19:4:293:LEU:HD11   | 19:4:316:PHE:HE1    | 1.61                     | 0.65              |
| 20:E:84:GLY:HA3     | 20:E:94:PHE:CE2     | 2.31                     | 0.65              |
| 22:I:289:LEU:HD23   | 22:I:296:ARG:NH2    | 2.10                     | 0.65              |
| 24:D40:94:ALA:CB    | 24:D40:543:MET:HE1  | 2.27                     | 0.65              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C32:847:ARG:HD2  | 10:C32:911:ILE:HD12  | 1.77                     | 0.65              |
| 10:C32:1488:ILE:CD1 | 10:C32:1528:LEU:HD23 | 2.26                     | 0.65              |
| 12:A48:374:PHE:CE2  | 12:A48:426:ILE:CD1   | 2.79                     | 0.65              |
| 2:M:627:TYR:OH      | 3:N:163:ALA:O        | 2.13                     | 0.65              |
| 7:Q:143:ARG:CZ      | 7:Q:147:GLU:OE2      | 2.44                     | 0.65              |
| 7:Q:297:VAL:HG13    | 7:Q:301:ARG:CD       | 2.23                     | 0.65              |
| 6:O16:119:ARG:HH21  | 6:O16:182:GLU:CB     | 2.08                     | 0.65              |
| 8:L8:608:PHE:CZ     | 8:L8:635:MET:CB      | 2.80                     | 0.65              |
| 8:L8:976:LEU:CD2    | 9:K8:1004:ARG:HE     | 2.02                     | 0.65              |
| 8:L16:621:SER:HB3   | 8:L16:657:TYR:CD1    | 2.32                     | 0.65              |
| 10:C16:389:LEU:HD23 | 10:C16:447:PHE:HE1   | 1.59                     | 0.65              |
| 10:C16:572:ILE:CG1  | 10:C16:606:MET:HE1   | 2.26                     | 0.65              |
| 10:C16:719:PRO:C    | 10:C16:721:PHE:H     | 2.05                     | 0.65              |
| 10:C16:1010:ALA:N   | 10:C16:1192:ARG:HH21 | 1.81                     | 0.65              |
| 11:A24:388:VAL:CG2  | 11:A24:459:ARG:HH12  | 2.09                     | 0.65              |
| 10:C24:1163:LEU:CD2 | 10:C24:1166:SER:CB   | 2.74                     | 0.65              |
| 11:A40:374:PHE:CE2  | 11:A40:426:ILE:CD1   | 2.79                     | 0.65              |
| 11:A40:388:VAL:CG2  | 11:A40:459:ARG:HH12  | 2.10                     | 0.65              |
| 10:C8:1002:LEU:HD12 | 10:C8:1019:ARG:HH12  | 1.61                     | 0.65              |
| 10:C8:1348:LEU:CD1  | 10:C8:1359:ILE:CG1   | 2.72                     | 0.65              |
| 11:A32:137:GLU:CD   | 18:B8:1901:GLN:HE22  | 2.05                     | 0.65              |
| 11:A32:270:VAL:CG1  | 11:A32:274:MET:HB3   | 2.25                     | 0.65              |
| 18:B:16:PHE:CZ      | 18:B:142:LEU:HD13    | 2.32                     | 0.65              |
| 18:B:266:ARG:HH12   | 18:B:383:PHE:HB3     | 1.61                     | 0.65              |
| 18:B:536:ILE:CG2    | 18:B:545:VAL:CG1     | 2.58                     | 0.65              |
| 18:B:1603:ASP:O     | 18:B:1606:LYS:HG3    | 1.96                     | 0.65              |
| 18:B8:496:LEU:CD2   | 18:B8:540:ILE:CD1    | 2.74                     | 0.65              |
| 18:B8:856:LEU:HD23  | 18:B8:860:HIS:HB2    | 1.75                     | 0.65              |
| 22:I16:289:LEU:CD2  | 22:I16:296:ARG:HH22  | 2.08                     | 0.65              |
| 24:D:94:ALA:CB      | 24:D:543:MET:HE1     | 2.26                     | 0.65              |
| 24:D32:749:ARG:NH1  | 24:D40:396:GLY:CA    | 2.54                     | 0.65              |
| 10:C32:300:VAL:HG12 | 10:C32:317:ARG:HG3   | 1.78                     | 0.65              |
| 10:C32:1824:ARG:O   | 10:C32:1828:THR:OG1  | 2.13                     | 0.65              |
| 2:M:385:LEU:HB3     | 2:M:388:SER:OG       | 1.97                     | 0.65              |
| 2:M16:385:LEU:HB3   | 2:M16:388:SER:OG     | 1.96                     | 0.65              |
| 2:M16:503:TYR:CE1   | 2:M16:507:LEU:CD1    | 2.79                     | 0.65              |
| 6:O:179:LYS:C       | 6:O:180:GLY:O        | 2.39                     | 0.65              |
| 5:P8:620:ILE:HG21   | 5:P8:660:ARG:NH2     | 2.12                     | 0.65              |
| 6:O16:291:SER:HB2   | 6:O16:293:MET:HE2    | 1.78                     | 0.65              |
| 10:C16:300:VAL:HG12 | 10:C16:317:ARG:HG3   | 1.78                     | 0.65              |
| 10:C16:647:GLU:OE1  | 10:C16:655:SER:HB3   | 1.95                     | 0.65              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:647:GLU:OE2   | 10:C16:656:THR:OG1   | 2.13                     | 0.65              |
| 10:C16:1163:LEU:CD2  | 10:C16:1166:SER:CB   | 2.74                     | 0.65              |
| 11:A24:103:GLU:OE1   | 21:H8:323:TYR:CZ     | 2.49                     | 0.65              |
| 10:C24:647:GLU:OE1   | 10:C24:655:SER:HB3   | 1.95                     | 0.65              |
| 10:C24:1336:ALA:C    | 10:C24:1338:ASP:H    | 2.04                     | 0.65              |
| 10:C24:1621:LYS:O    | 10:C24:1622:SER:C    | 2.35                     | 0.65              |
| 10:C24:1708:ARG:NH1  | 21:H24:279:GLU:OE2   | 2.17                     | 0.65              |
| 10:C:717:GLU:O       | 10:C:719:PRO:CD      | 2.44                     | 0.65              |
| 10:C:1824:ARG:O      | 10:C:1828:THR:OG1    | 2.13                     | 0.65              |
| 10:C8:499:LEU:HD21   | 10:C8:505:PHE:HZ     | 1.60                     | 0.65              |
| 10:C8:963:GLN:HG2    | 10:C8:1138:GLU:O     | 1.97                     | 0.65              |
| 11:A32:707:LEU:HD21  | 11:A32:767:ARG:HH22  | 1.59                     | 0.65              |
| 18:B:171:ILE:HD13    | 18:B:226:TYR:CB      | 2.25                     | 0.65              |
| 18:B:286:GLN:OE1     | 18:B:443:PHE:CG      | 2.49                     | 0.65              |
| 18:B:917:PHE:HE2     | 18:B:960:GLN:CD      | 2.05                     | 0.65              |
| 18:B:1788:ILE:O      | 18:B:1789:THR:C      | 2.26                     | 0.65              |
| 18:B8:195:MET:SD     | 18:B8:199:LEU:HD23   | 2.36                     | 0.65              |
| 18:B8:671:MET:HE3    | 18:B8:736:ALA:HB3    | 1.76                     | 0.65              |
| 20:E:353:ILE:HD13    | 20:E:413:PHE:HD2     | 0.69                     | 0.65              |
| 20:E8:434:TRP:CE2    | 24:D40:72:GLU:OE2    | 2.50                     | 0.65              |
| 20:E8:434:TRP:C      | 20:E8:436:THR:N      | 2.55                     | 0.65              |
| 21:H24:322:LEU:CD1   | 23:J24:689:LEU:HD23  | 2.24                     | 0.65              |
| 10:C32:1424:GLN:HE21 | 10:C32:1478:VAL:CG1  | 2.10                     | 0.65              |
| 1:R:1290:ILE:HD13    | 10:C:605:GLU:CD      | 2.20                     | 0.65              |
| 2:M8:385:LEU:HB3     | 2:M8:388:SER:OG      | 1.97                     | 0.65              |
| 2:M8:414:GLY:HA2     | 8:L8:401:LYS:NZ      | 2.11                     | 0.65              |
| 2:M16:377:ARG:HH12   | 2:M16:477:ASP:HB2    | 1.61                     | 0.65              |
| 2:M16:569:LEU:HD23   | 3:N16:287:LYS:CD     | 2.27                     | 0.65              |
| 2:M16:625:HIS:CD2    | 3:N16:225:PRO:HB3    | 2.30                     | 0.65              |
| 6:O:291:SER:HB2      | 6:O:293:MET:HE2      | 1.77                     | 0.65              |
| 10:C16:499:LEU:HD21  | 10:C16:505:PHE:HZ    | 1.60                     | 0.65              |
| 10:C16:1665:THR:HG23 | 10:C24:1601:TYR:C    | 2.22                     | 0.65              |
| 11:A24:468:VAL:HG22  | 24:D16:1103:LEU:HD12 | 0.65                     | 0.65              |
| 10:C24:499:LEU:HD21  | 10:C24:505:PHE:HZ    | 1.60                     | 0.65              |
| 10:C:407:LYS:HG3     | 10:C:465:PHE:CE1     | 2.31                     | 0.65              |
| 10:C:499:LEU:HD21    | 10:C:505:PHE:HZ      | 1.60                     | 0.65              |
| 10:C8:647:GLU:OE2    | 10:C8:656:THR:OG1    | 2.13                     | 0.65              |
| 11:A16:36:ASN:HD21   | 22:I:293:LYS:HE2     | 1.52                     | 0.65              |
| 11:A16:326:TYR:OH    | 17:F8:74:ILE:O       | 2.12                     | 0.65              |
| 11:A16:674:GLY:HA3   | 24:D16:1396:PRO:HG3  | 1.78                     | 0.65              |
| 11:A32:374:PHE:CE2   | 11:A32:426:ILE:CD1   | 2.79                     | 0.65              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:177:ARG:HG3     | 18:B:233:ARG:HH21    | 1.61                     | 0.65              |
| 18:B:496:LEU:CD2     | 18:B:540:ILE:CD1     | 2.74                     | 0.65              |
| 18:B:690:TRP:CZ3     | 18:B:739:VAL:CG2     | 2.79                     | 0.65              |
| 18:B:750:GLU:CG      | 18:B:760:ARG:CZ      | 2.73                     | 0.65              |
| 18:B:1045:LYS:NZ     | 18:B:1100:LEU:HD21   | 2.11                     | 0.65              |
| 18:B8:16:PHE:CZ      | 18:B8:142:LEU:HD13   | 2.32                     | 0.65              |
| 21:H16:322:LEU:CD1   | 23:J16:689:LEU:HD23  | 2.24                     | 0.65              |
| 24:D16:94:ALA:CB     | 24:D16:543:MET:HE1   | 2.27                     | 0.65              |
| 24:D40:839:GLU:C     | 24:D40:971:HIS:CE1   | 2.75                     | 0.65              |
| 10:C32:499:LEU:HD21  | 10:C32:505:PHE:HZ    | 1.60                     | 0.65              |
| 10:C32:717:GLU:O     | 10:C32:719:PRO:CD    | 2.44                     | 0.65              |
| 10:C32:1111:SER:C    | 10:C32:1113:LYS:H    | 2.05                     | 0.65              |
| 1:R:1424:LYS:NZ      | 6:O:105:ASN:HD22     | 1.90                     | 0.65              |
| 2:M:188:ARG:HB2      | 3:N:264:ARG:HH11     | 1.62                     | 0.65              |
| 2:M:627:TYR:OH       | 3:N:162:THR:HB       | 1.97                     | 0.65              |
| 2:M:772:PHE:CE1      | 2:M:776:LEU:HD11     | 2.32                     | 0.65              |
| 1:R16:1075:LYS:HE2   | 5:P16:713:LEU:C      | 2.21                     | 0.65              |
| 5:P:109:ILE:HG12     | 14:W:18:PRO:HG2      | 1.40                     | 0.65              |
| 5:P8:506:ASN:ND2     | 7:Q8:198:TYR:OH      | 2.30                     | 0.65              |
| 5:P8:615:HIS:N       | 5:P8:629:ARG:NH1     | 2.45                     | 0.65              |
| 10:C16:1074:LEU:CG   | 10:C16:1075:ASP:N    | 2.59                     | 0.65              |
| 10:C16:1358:ASP:C    | 10:C16:1360:GLN:N    | 2.53                     | 0.65              |
| 10:C16:1824:ARG:O    | 10:C16:1828:THR:OG1  | 2.13                     | 0.65              |
| 10:C24:1814:LYS:HZ3  | 23:J24:738:MET:HB2   | 1.56                     | 0.65              |
| 11:A40:607:ARG:NH1   | 24:D32:914:PHE:HE1   | 1.94                     | 0.65              |
| 13:V:815:TYR:HH      | 15:J:627:ILE:HD11    | 1.60                     | 0.65              |
| 10:C:300:VAL:HG12    | 10:C:317:ARG:HG3     | 1.77                     | 0.65              |
| 10:C:983:SER:CB      | 10:C:1040:HIS:CD2    | 2.80                     | 0.65              |
| 10:C8:168:ARG:NH1    | 10:C8:229:PRO:CA     | 2.58                     | 0.65              |
| 10:C8:1133:ILE:HG12  | 10:C8:1152:LYS:HD2   | 1.79                     | 0.65              |
| 10:C8:1163:LEU:CD2   | 10:C8:1166:SER:CB    | 2.74                     | 0.65              |
| 11:A32:159:LYS:NZ    | 18:B8:1918:ARG:HG3   | 2.12                     | 0.65              |
| 18:B:202:LEU:CD1     | 18:B:820:ARG:NH1     | 2.60                     | 0.65              |
| 18:B:968:PHE:HB2     | 18:B:1040:MET:HE1    | 1.76                     | 0.65              |
| 18:B:1209:LEU:HD13   | 18:B:1266:LEU:HD21   | 1.77                     | 0.65              |
| 18:B8:86:LYS:CD      | 18:B8:123:LEU:HD11   | 2.25                     | 0.65              |
| 18:B8:1209:LEU:HD13  | 18:B8:1266:LEU:HD21  | 1.77                     | 0.65              |
| 18:B8:1603:ASP:O     | 18:B8:1606:LYS:HG3   | 1.96                     | 0.65              |
| 24:D16:275:LYS:HE3   | 24:D16:294:GLU:CD    | 2.21                     | 0.65              |
| 10:C32:450:PRO:C     | 10:C32:452:LEU:HD23  | 2.22                     | 0.65              |
| 10:C32:1002:LEU:HD12 | 10:C32:1019:ARG:HH12 | 1.61                     | 0.65              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:HB    | 1.97                     | 0.65              |
| 2:M:377:ARG:NH1      | 2:M:477:ASP:HB2     | 2.11                     | 0.65              |
| 1:R8:1442:THR:HG21   | 3:N8:13:ILE:HD11    | 1.77                     | 0.65              |
| 2:M8:348:GLU:O       | 2:M8:350:SER:N      | 2.29                     | 0.65              |
| 2:M16:188:ARG:HB2    | 3:N16:264:ARG:HH11  | 1.62                     | 0.65              |
| 2:M16:351:ALA:CB     | 8:L16:219:ILE:HG23  | 2.26                     | 0.65              |
| 2:M16:772:PHE:CE1    | 2:M16:776:LEU:HD11  | 2.32                     | 0.65              |
| 5:P:206:SER:HG       | 5:P:207:HIS:CE1     | 2.14                     | 0.65              |
| 7:Q:272:SER:C        | 7:Q:274:ASN:H       | 2.05                     | 0.65              |
| 7:Q:295:SER:C        | 7:Q:297:VAL:N       | 2.54                     | 0.65              |
| 5:P8:101:LEU:HD21    | 5:P8:133:TYR:CG     | 2.31                     | 0.65              |
| 5:P16:105:ARG:HG2    | 5:P16:126:TRP:HZ2   | 1.62                     | 0.65              |
| 9:K:1074:ARG:CD      | 9:K:1126:LEU:CD2    | 2.71                     | 0.65              |
| 10:C16:300:VAL:HG12  | 10:C16:317:ARG:CG   | 2.27                     | 0.65              |
| 10:C16:743:PHE:CZ    | 10:C16:749:LEU:HD23 | 2.32                     | 0.65              |
| 10:C16:1336:ALA:C    | 10:C16:1338:ASP:H   | 2.04                     | 0.65              |
| 11:A24:342:VAL:CG1   | 17:F:77:TYR:CE1     | 2.78                     | 0.65              |
| 10:C24:1074:LEU:HD23 | 18:B8:256:VAL:C     | 2.22                     | 0.65              |
| 10:C24:1358:ASP:C    | 10:C24:1360:GLN:N   | 2.53                     | 0.65              |
| 12:A:642:GLY:N       | 12:A:685:ARG:NH2    | 2.44                     | 0.65              |
| 10:C:1622:SER:OG     | 10:C:1623:ILE:N     | 2.08                     | 0.65              |
| 10:C8:1297:HIS:NE2   | 10:C8:1372:ALA:HB1  | 2.11                     | 0.65              |
| 18:B:1657:TYR:CE2    | 18:B:1658:MET:HG2   | 2.31                     | 0.65              |
| 18:B8:202:LEU:CD1    | 18:B8:820:ARG:NH1   | 2.59                     | 0.65              |
| 18:B8:690:TRP:CZ3    | 18:B8:739:VAL:CG2   | 2.79                     | 0.65              |
| 20:E:434:TRP:C       | 20:E:436:THR:N      | 2.55                     | 0.65              |
| 20:E8:433:LYS:C      | 20:E8:435:ALA:H     | 2.02                     | 0.65              |
| 22:I:203:GLN:HB3     | 22:I:209:TRP:CH2    | 2.32                     | 0.65              |
| 21:H24:262:GLU:CD    | 23:J24:648:TYR:OH   | 2.39                     | 0.65              |
| 10:C32:57:VAL:HA     | 10:C32:62:ILE:HD11  | 1.77                     | 0.65              |
| 10:C32:389:LEU:HD23  | 10:C32:447:PHE:HE1  | 1.59                     | 0.65              |
| 10:C32:572:ILE:HD13  | 10:C32:606:MET:HE2  | 1.70                     | 0.65              |
| 10:C32:719:PRO:C     | 10:C32:721:PHE:H    | 2.05                     | 0.65              |
| 10:C32:1129:VAL:HG12 | 10:C32:1130:SER:N   | 2.11                     | 0.65              |
| 1:R8:1191:LYS:O      | 1:R8:1192:LYS:C     | 2.35                     | 0.65              |
| 2:M8:310:HIS:HA      | 2:M8:313:MET:HE2    | 1.78                     | 0.65              |
| 2:M8:349:ASP:O       | 2:M8:351:ALA:N      | 2.28                     | 0.65              |
| 2:M8:351:ALA:CB      | 8:L8:219:ILE:HG22   | 2.22                     | 0.65              |
| 2:M8:772:PHE:CE1     | 2:M8:776:LEU:HD11   | 2.32                     | 0.65              |
| 2:M16:367:SER:HB2    | 2:M16:486:MET:HE1   | 1.78                     | 0.65              |
| 2:M16:851:LEU:HD22   | 4:T16:653:GLN:HE21  | 1.62                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:O:119:ARG:HH22    | 6:O:182:GLU:HG2     | 1.59                     | 0.65              |
| 8:L:1041:SER:CB     | 8:L:1054:HIS:HE1    | 1.92                     | 0.65              |
| 9:K:614:PHE:HA      | 9:K:683:GLN:NE2     | 2.11                     | 0.65              |
| 9:K:923:ILE:HG22    | 9:K:929:ARG:NE      | 2.11                     | 0.65              |
| 9:K:1154:TRP:CH2    | 9:K:1219:VAL:HG12   | 2.32                     | 0.65              |
| 11:A24:36:ASN:HD22  | 22:I8:293:LYS:HZ1   | 1.44                     | 0.65              |
| 11:A24:374:PHE:CE2  | 11:A24:426:ILE:CD1  | 2.79                     | 0.65              |
| 10:C24:398:SER:HA   | 10:C24:458:VAL:HG11 | 1.77                     | 0.65              |
| 12:A:634:ILE:HG21   | 12:A:678:LYS:HZ2    | 1.62                     | 0.65              |
| 14:W:645:HIS:HE1    | 15:J:572:ASP:OD1    | 1.80                     | 0.65              |
| 10:C8:798:VAL:CG1   | 10:C8:802:TRP:CE2   | 2.80                     | 0.65              |
| 10:C8:1050:HIS:CD2  | 10:C8:1086:LYS:HZ1  | 1.94                     | 0.65              |
| 10:C8:1212:GLU:OE1  | 16:A8:109:HIS:NE2   | 2.26                     | 0.65              |
| 11:A16:374:PHE:CE2  | 11:A16:426:ILE:CD1  | 2.79                     | 0.65              |
| 18:B:771:MET:HE3    | 18:B:840:VAL:HG21   | 1.79                     | 0.65              |
| 18:B8:266:ARG:HH12  | 18:B8:383:PHE:HB3   | 1.61                     | 0.65              |
| 21:H:162:LYS:NZ     | 21:H:168:ASP:OD1    | 2.30                     | 0.65              |
| 22:I:199:PHE:CE1    | 23:J32:620:MET:HG3  | 2.31                     | 0.65              |
| 22:I:289:LEU:CD2    | 22:I:296:ARG:HH22   | 2.07                     | 0.65              |
| 21:H8:162:LYS:NZ    | 21:H8:168:ASP:OD1   | 2.30                     | 0.65              |
| 21:H8:207:GLN:NE2   | 23:J8:572:ASP:OD1   | 2.26                     | 0.65              |
| 21:H8:262:GLU:CD    | 23:J8:648:TYR:OH    | 2.39                     | 0.65              |
| 10:C32:249:THR:O    | 10:C32:251:GLY:N    | 2.30                     | 0.65              |
| 10:C32:593:ARG:HH12 | 10:C32:655:SER:HG   | 1.41                     | 0.65              |
| 10:C32:878:ARG:HH21 | 10:C32:885:VAL:CG2  | 2.09                     | 0.65              |
| 10:C32:1265:ARG:C   | 10:C32:1268:ARG:HG2 | 2.19                     | 0.65              |
| 10:C32:1439:ILE:CD1 | 10:C32:1457:LEU:CD1 | 2.75                     | 0.65              |
| 2:M8:627:TYR:OH     | 3:N8:163:ALA:O      | 2.14                     | 0.64              |
| 5:P:281:ILE:HD11    | 5:P:341:MET:HE2     | 1.78                     | 0.64              |
| 5:P8:157:SER:O      | 5:P8:251:LYS:NZ     | 2.22                     | 0.64              |
| 5:P8:303:LYS:HG3    | 5:P8:373:PHE:CE1    | 2.33                     | 0.64              |
| 8:L8:1064:ASP:CG    | 9:K8:1101:GLU:OE1   | 2.39                     | 0.64              |
| 9:K:751:LEU:HD22    | 9:K:754:ARG:HD3     | 1.76                     | 0.64              |
| 9:K8:649:MET:HB3    | 9:K8:704:ARG:HH22   | 1.55                     | 0.64              |
| 10:C16:798:VAL:CG1  | 10:C16:802:TRP:CE2  | 2.80                     | 0.64              |
| 10:C16:1814:LYS:NZ  | 23:J32:738:MET:SD   | 2.70                     | 0.64              |
| 10:C24:300:VAL:HG12 | 10:C24:317:ARG:CG   | 2.27                     | 0.64              |
| 10:C24:389:LEU:HD23 | 10:C24:447:PHE:HE1  | 1.59                     | 0.64              |
| 13:V:804:VAL:HG13   | 14:W:695:LEU:CD1    | 2.27                     | 0.64              |
| 10:C:300:VAL:HG12   | 10:C:317:ARG:CG     | 2.27                     | 0.64              |
| 11:A16:137:GLU:CD   | 18:B:1901:GLN:HE22  | 2.05                     | 0.64              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:262:HIS:ND1     | 18:B:379:LEU:CD2     | 2.54                     | 0.64              |
| 18:B:1529:GLU:OE1    | 24:D16:1411:ASN:HB3  | 1.97                     | 0.64              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:CB     | 2.75                     | 0.64              |
| 21:H8:322:LEU:CD1    | 23:J8:689:LEU:HD23   | 2.24                     | 0.64              |
| 22:I24:199:PHE:CD1   | 23:J24:620:MET:CG    | 2.76                     | 0.64              |
| 22:I24:289:LEU:HD23  | 22:I24:296:ARG:NH2   | 2.10                     | 0.64              |
| 21:H16:162:LYS:NZ    | 21:H16:168:ASP:OD1   | 2.30                     | 0.64              |
| 10:C32:572:ILE:CG1   | 10:C32:606:MET:HE1   | 2.26                     | 0.64              |
| 10:C32:1297:HIS:NE2  | 10:C32:1372:ALA:HB1  | 2.12                     | 0.64              |
| 10:C32:1339:VAL:HG13 | 10:C32:1742:CYS:HB3  | 1.80                     | 0.64              |
| 10:C32:1716:LYS:HG3  | 10:C32:1721:GLN:HE21 | 1.61                     | 0.64              |
| 2:M:851:LEU:HD22     | 4:T:653:GLN:HE21     | 1.62                     | 0.64              |
| 7:Q:327:LEU:CD1      | 7:Q:358:PHE:CE1      | 2.76                     | 0.64              |
| 5:P8:105:ARG:HH22    | 5:P8:133:TYR:CB      | 2.09                     | 0.64              |
| 7:Q8:241:HIS:HA      | 7:Q8:257:LEU:HD12    | 1.79                     | 0.64              |
| 5:P16:303:LYS:HG3    | 5:P16:373:PHE:CE1    | 2.32                     | 0.64              |
| 5:P16:506:ASN:ND2    | 7:Q16:198:TYR:OH     | 2.30                     | 0.64              |
| 8:L16:177:ARG:CG     | 12:A48:744:GLU:OE1   | 2.43                     | 0.64              |
| 10:C16:398:SER:HA    | 10:C16:458:VAL:HG11  | 1.78                     | 0.64              |
| 10:C16:450:PRO:C     | 10:C16:452:LEU:HD23  | 2.22                     | 0.64              |
| 10:C16:1230:TYR:CE2  | 10:C16:1295:ALA:HB1  | 2.33                     | 0.64              |
| 10:C16:1547:LYS:HD3  | 24:D8:1406:SER:H     | 0.71                     | 0.64              |
| 10:C24:878:ARG:HH21  | 10:C24:885:VAL:CG2   | 2.09                     | 0.64              |
| 12:A:374:PHE:HE2     | 12:A:426:ILE:HD12    | 1.61                     | 0.64              |
| 10:C:798:VAL:CG1     | 10:C:802:TRP:CE2     | 2.80                     | 0.64              |
| 10:C8:578:LEU:HB3    | 10:C8:584:ILE:CD1    | 2.27                     | 0.64              |
| 11:A16:159:LYS:NZ    | 18:B:1918:ARG:HG3    | 2.12                     | 0.64              |
| 11:A16:388:VAL:CG2   | 11:A16:459:ARG:HH12  | 2.09                     | 0.64              |
| 18:B:235:ARG:NH1     | 18:B:308:GLU:HB3     | 2.12                     | 0.64              |
| 18:B8:982:SER:OG     | 18:B8:983:ARG:N      | 2.31                     | 0.64              |
| 18:B8:1175:ALA:HB1   | 18:B8:1272:TRP:HD1   | 1.58                     | 0.64              |
| 19:4:180:ALA:HB3     | 19:4:202:ILE:CD1     | 2.13                     | 0.64              |
| 21:H:262:GLU:CD      | 23:J32:648:TYR:OH    | 2.39                     | 0.64              |
| 23:J32:718:GLN:O     | 23:J32:722:LEU:HD12  | 1.98                     | 0.64              |
| 22:I8:298:ALA:HB1    | 22:I8:303:SER:OG     | 1.97                     | 0.64              |
| 10:C32:578:LEU:HB3   | 10:C32:584:ILE:CD1   | 2.27                     | 0.64              |
| 10:C32:668:ALA:HA    | 10:C32:700:MET:HE3   | 1.76                     | 0.64              |
| 1:R:1033:LYS:CE      | 24:D:1436:ARG:CZ     | 2.74                     | 0.64              |
| 2:M8:367:SER:HB2     | 2:M8:486:MET:HE1     | 1.78                     | 0.64              |
| 3:N16:267:TRP:HH2    | 3:N16:294:TRP:HH2    | 1.43                     | 0.64              |
| 6:O:9:ASP:OD2        | 6:O:51:LYS:HE2       | 1.97                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:O8:9:ASP:OD2      | 6:O8:51:LYS:HE2     | 1.97                     | 0.64              |
| 5:P16:105:ARG:NH2   | 5:P16:133:TYR:HD1   | 1.49                     | 0.64              |
| 7:Q16:295:SER:CB    | 7:Q16:297:VAL:HG23  | 2.27                     | 0.64              |
| 9:K8:751:LEU:HD22   | 9:K8:754:ARG:NH1    | 2.12                     | 0.64              |
| 10:C16:667:ILE:CG2  | 10:C16:670:GLU:N    | 2.59                     | 0.64              |
| 11:A24:43:LEU:HD23  | 23:J8:700:LEU:CD2   | 2.27                     | 0.64              |
| 10:C:848:CYS:CA     | 10:C:906:ARG:HH22   | 1.97                     | 0.64              |
| 10:C8:878:ARG:HH21  | 10:C8:885:VAL:CG2   | 2.09                     | 0.64              |
| 10:C8:1055:GLU:O    | 10:C8:1057:THR:N    | 2.30                     | 0.64              |
| 11:A16:154:ILE:HG23 | 18:B:1851:VAL:CG2   | 2.28                     | 0.64              |
| 11:A32:374:PHE:HE2  | 11:A32:426:ILE:HD12 | 1.60                     | 0.64              |
| 18:B:671:MET:HE1    | 18:B:736:ALA:CB     | 2.27                     | 0.64              |
| 19:48:281:TRP:CE3   | 19:48:288:SER:HB3   | 2.32                     | 0.64              |
| 22:I:298:ALA:HB1    | 22:I:303:SER:OG     | 1.97                     | 0.64              |
| 23:J8:718:GLN:O     | 23:J8:722:LEU:HD12  | 1.98                     | 0.64              |
| 22:I24:203:GLN:HB3  | 22:I24:209:TRP:CZ2  | 2.32                     | 0.64              |
| 24:D:308:ASN:ND2    | 24:D16:753:ARG:CD   | 2.60                     | 0.64              |
| 24:D24:275:LYS:HE3  | 24:D24:294:GLU:CD   | 2.21                     | 0.64              |
| 10:C32:667:ILE:HD12 | 10:C32:700:MET:HE1  | 1.76                     | 0.64              |
| 2:M:772:PHE:CE1     | 2:M:776:LEU:CD1     | 2.80                     | 0.64              |
| 5:P16:510:ILE:HD11  | 7:Q16:183:ARG:HH12  | 1.63                     | 0.64              |
| 8:L:1096:GLU:HG2    | 9:K:998:GLN:NE2     | 2.12                     | 0.64              |
| 11:A24:374:PHE:HE2  | 11:A24:426:ILE:HD12 | 1.60                     | 0.64              |
| 10:C24:798:VAL:CG1  | 10:C24:802:TRP:CE2  | 2.80                     | 0.64              |
| 12:A:374:PHE:CE2    | 12:A:426:ILE:CD1    | 2.80                     | 0.64              |
| 13:V:861:PHE:CB     | 14:W:741:ARG:NH2    | 2.59                     | 0.64              |
| 14:W:711:ARG:CD     | 10:C8:1609:ASP:CB   | 2.74                     | 0.64              |
| 10:C:743:PHE:CZ     | 10:C:749:LEU:HD23   | 2.32                     | 0.64              |
| 10:C:1111:SER:C     | 10:C:1113:LYS:H     | 2.05                     | 0.64              |
| 18:B:1377:ASP:OD2   | 18:B:1381:ARG:NH2   | 2.30                     | 0.64              |
| 18:B8:113:TYR:CE1   | 18:B8:119:VAL:CG1   | 2.81                     | 0.64              |
| 19:48:293:LEU:HD11  | 19:48:316:PHE:HE1   | 1.61                     | 0.64              |
| 24:D24:94:ALA:CB    | 24:D24:543:MET:HE1  | 2.27                     | 0.64              |
| 10:C32:275:ALA:HB1  | 10:C32:326:LEU:CD1  | 2.27                     | 0.64              |
| 10:C32:798:VAL:CG1  | 10:C32:802:TRP:CE2  | 2.80                     | 0.64              |
| 10:C32:847:ARG:CZ   | 10:C32:911:ILE:N    | 2.57                     | 0.64              |
| 10:C32:1055:GLU:O   | 10:C32:1057:THR:N   | 2.30                     | 0.64              |
| 10:C32:1230:TYR:CE2 | 10:C32:1295:ALA:HB1 | 2.33                     | 0.64              |
| 12:A48:638:LEU:HD21 | 12:A48:663:LEU:HD21 | 1.80                     | 0.64              |
| 2:M:385:LEU:HD11    | 2:M:396:PHE:HE2     | 1.58                     | 0.64              |
| 1:R8:1266:THR:HA    | 5:P8:684:ARG:HH21   | 0.69                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M8:627:TYR:CD1    | 2:M8:627:TYR:N      | 2.61                     | 0.64              |
| 2:M16:417:ARG:HD3   | 8:L16:298:PHE:CE2   | 2.30                     | 0.64              |
| 5:P:620:ILE:HG21    | 5:P:660:ARG:NH2     | 2.12                     | 0.64              |
| 5:P8:281:ILE:HD11   | 5:P8:341:MET:HE2    | 1.78                     | 0.64              |
| 6:O8:179:LYS:C      | 6:O8:180:GLY:O      | 2.39                     | 0.64              |
| 9:K:975:MET:SD      | 9:K:989:VAL:HG11    | 2.37                     | 0.64              |
| 10:C24:249:THR:O    | 10:C24:251:GLY:N    | 2.30                     | 0.64              |
| 10:C24:300:VAL:HG12 | 10:C24:317:ARG:HG3  | 1.77                     | 0.64              |
| 10:C24:743:PHE:CZ   | 10:C24:749:LEU:HD23 | 2.32                     | 0.64              |
| 11:A40:465:SER:HB3  | 24:D32:1100:GLN:NE2 | 2.05                     | 0.64              |
| 12:A:842:ALA:O      | 12:A:845:THR:HG23   | 1.96                     | 0.64              |
| 14:W:631:TYR:CE2    | 15:J:554:LEU:CD2    | 2.69                     | 0.64              |
| 10:C:557:VAL:HG22   | 10:C:565:ARG:CZ     | 2.27                     | 0.64              |
| 10:C:1133:ILE:HG12  | 10:C:1152:LYS:HD2   | 1.79                     | 0.64              |
| 10:C:1230:TYR:CE2   | 10:C:1295:ALA:HB1   | 2.33                     | 0.64              |
| 10:C8:169:GLN:OE1   | 10:C8:169:GLN:CA    | 2.44                     | 0.64              |
| 10:C8:1336:ALA:C    | 10:C8:1338:ASP:H    | 2.04                     | 0.64              |
| 10:C8:1716:LYS:HG3  | 10:C8:1721:GLN:HE21 | 1.61                     | 0.64              |
| 18:B:268:GLN:HE22   | 18:B:323:GLU:CB     | 2.11                     | 0.64              |
| 18:B:978:ASN:O      | 18:B:980:LYS:N      | 2.30                     | 0.64              |
| 18:B:982:SER:OG     | 18:B:983:ARG:N      | 2.30                     | 0.64              |
| 18:B:1121:ALA:O     | 18:B:1122:SER:C     | 2.35                     | 0.64              |
| 20:E8:85:LEU:O      | 20:E8:89:LEU:CD1    | 2.45                     | 0.64              |
| 21:H:322:LEU:CD1    | 23:J32:689:LEU:HD23 | 2.24                     | 0.64              |
| 22:I8:289:LEU:CD2   | 22:I8:296:ARG:HH22  | 2.07                     | 0.64              |
| 23:J24:718:GLN:O    | 23:J24:722:LEU:HD12 | 1.98                     | 0.64              |
| 10:C32:300:VAL:HG12 | 10:C32:317:ARG:CG   | 2.27                     | 0.64              |
| 10:C32:562:PRO:HA   | 10:C32:565:ARG:NE   | 2.13                     | 0.64              |
| 2:M:310:HIS:HA      | 2:M:313:MET:HE2     | 1.78                     | 0.64              |
| 2:M:569:LEU:HD23    | 3:N:287:LYS:CD      | 2.27                     | 0.64              |
| 2:M16:348:GLU:O     | 2:M16:350:SER:N     | 2.29                     | 0.64              |
| 2:M16:772:PHE:CE1   | 2:M16:776:LEU:CD1   | 2.80                     | 0.64              |
| 5:P:506:ASN:ND2     | 7:Q:198:TYR:OH      | 2.30                     | 0.64              |
| 5:P8:247:GLU:OE1    | 5:P8:296:PHE:N      | 2.29                     | 0.64              |
| 7:Q8:241:HIS:CD2    | 7:Q8:258:ARG:HE     | 2.16                     | 0.64              |
| 10:C16:962:PHE:CE2  | 10:C16:997:ILE:HD13 | 2.33                     | 0.64              |
| 10:C16:1055:GLU:O   | 10:C16:1057:THR:N   | 2.30                     | 0.64              |
| 14:W:1:MET:CE       | 10:C:1497:LYS:HD3   | 2.16                     | 0.64              |
| 11:A16:148:LEU:CD1  | 18:B:1956:ILE:HD12  | 2.24                     | 0.64              |
| 18:B:113:TYR:CE1    | 18:B:119:VAL:CG1    | 2.81                     | 0.64              |
| 18:B:1256:THR:HG23  | 24:D16:1238:GLU:CG  | 2.20                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:1839:GLU:O     | 18:B:1843:THR:OG1   | 2.15                     | 0.64              |
| 18:B8:978:ASN:O     | 18:B8:980:LYS:N     | 2.30                     | 0.64              |
| 19:48:180:ALA:HB3   | 19:48:202:ILE:CD1   | 2.13                     | 0.64              |
| 22:I8:196:VAL:HA    | 23:J8:620:MET:HE1   | 0.69                     | 0.64              |
| 21:H24:154:VAL:HG13 | 21:H24:188:ARG:HG2  | 1.80                     | 0.64              |
| 22:I16:298:ALA:HB1  | 22:I16:303:SER:OG   | 1.97                     | 0.64              |
| 10:C32:1220:SER:O   | 10:C32:1225:ARG:NH2 | 2.31                     | 0.64              |
| 1:R8:1079:ASP:OD1   | 5:P8:713:LEU:HD22   | 1.97                     | 0.64              |
| 1:R8:1249:SER:HB2   | 1:R8:1280:GLU:CD    | 2.22                     | 0.64              |
| 1:R8:1449:TRP:HH2   | 2:M8:161:ASP:C      | 2.06                     | 0.64              |
| 2:M8:451:PHE:O      | 8:L8:295:HIS:HD2    | 1.81                     | 0.64              |
| 2:M8:503:TYR:CE1    | 2:M8:507:LEU:HD12   | 2.33                     | 0.64              |
| 2:M8:569:LEU:HD23   | 3:N8:287:LYS:CD     | 2.27                     | 0.64              |
| 2:M8:763:ASP:OD1    | 2:M8:818:THR:HG23   | 1.98                     | 0.64              |
| 3:N8:267:TRP:CH2    | 3:N8:294:TRP:CH2    | 2.86                     | 0.64              |
| 5:P:109:ILE:HG21    | 14:W:18:PRO:HG2     | 1.73                     | 0.64              |
| 7:Q8:295:SER:CB     | 7:Q8:297:VAL:HG23   | 2.27                     | 0.64              |
| 5:P16:402:LEU:CD1   | 5:P16:433:LEU:HD13  | 2.28                     | 0.64              |
| 7:Q16:325:GLU:OE1   | 7:Q16:328:ALA:HB2   | 1.97                     | 0.64              |
| 9:K8:1154:TRP:CH2   | 9:K8:1219:VAL:HG12  | 2.32                     | 0.64              |
| 10:C16:225:LEU:HD22 | 10:C16:388:TYR:OH   | 1.96                     | 0.64              |
| 10:C16:275:ALA:HB1  | 10:C16:326:LEU:CD1  | 2.28                     | 0.64              |
| 10:C24:182:ASP:HB2  | 10:C24:183:PRO:CD   | 2.23                     | 0.64              |
| 10:C24:1297:HIS:NE2 | 10:C24:1372:ALA:HB1 | 2.11                     | 0.64              |
| 13:V:773:LEU:HD21   | 15:J:582:LEU:HD13   | 1.80                     | 0.64              |
| 10:C:719:PRO:C      | 10:C:721:PHE:H      | 2.05                     | 0.64              |
| 10:C:1290:HIS:CB    | 10:C:1334:MET:CE    | 2.72                     | 0.64              |
| 10:C:1621:LYS:O     | 10:C:1622:SER:C     | 2.35                     | 0.64              |
| 10:C8:275:ALA:HB1   | 10:C8:326:LEU:CD1   | 2.28                     | 0.64              |
| 10:C8:572:ILE:CG1   | 10:C8:606:MET:HE1   | 2.26                     | 0.64              |
| 10:C8:743:PHE:CZ    | 10:C8:749:LEU:HD23  | 2.32                     | 0.64              |
| 11:A16:374:PHE:HE2  | 11:A16:426:ILE:HD12 | 1.60                     | 0.64              |
| 11:A32:388:VAL:CG2  | 11:A32:459:ARG:HH12 | 2.09                     | 0.64              |
| 18:B:344:LYS:HE3    | 18:B:350:LEU:O      | 1.96                     | 0.64              |
| 18:B8:1161:LEU:HD11 | 18:B8:1403:ILE:CB   | 2.28                     | 0.64              |
| 20:E:447:ILE:HG23   | 20:E:451:ILE:HG21   | 1.80                     | 0.64              |
| 20:E8:84:GLY:HA3    | 20:E8:94:PHE:CE2    | 2.31                     | 0.64              |
| 21:H24:162:LYS:NZ   | 21:H24:168:ASP:OD1  | 2.30                     | 0.64              |
| 22:I16:203:GLN:HB3  | 22:I16:209:TRP:CZ2  | 2.32                     | 0.64              |
| 10:C32:390:HIS:CB   | 10:C32:452:LEU:HB2  | 2.24                     | 0.64              |
| 2:M:763:ASP:OD1     | 2:M:818:THR:HG23    | 1.98                     | 0.64              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M8:448:ASP:OD1     | 2:M8:448:ASP:N      | 2.21                     | 0.64              |
| 2:M8:772:PHE:CE1     | 2:M8:776:LEU:CD1    | 2.80                     | 0.64              |
| 2:M16:755:THR:HB     | 2:M16:757:VAL:HG23  | 1.79                     | 0.64              |
| 7:Q:241:HIS:HA       | 7:Q:257:LEU:HD12    | 1.78                     | 0.64              |
| 9:K:635:ALA:CA       | 9:K:655:GLN:NE2     | 2.26                     | 0.64              |
| 9:K:853:ALA:HB2      | 9:K:856:ILE:HD12    | 1.80                     | 0.64              |
| 10:C16:1547:LYS:HE2  | 24:D8:1405:GLY:N    | 2.13                     | 0.64              |
| 10:C24:904:ILE:HD11  | 10:C24:964:LEU:HD12 | 1.80                     | 0.64              |
| 10:C24:1424:GLN:HE21 | 10:C24:1478:VAL:CG1 | 2.09                     | 0.64              |
| 11:A40:33:LEU:CD2    | 22:I16:286:LEU:HD13 | 2.27                     | 0.64              |
| 12:A:440:LEU:HD12    | 12:A:443:LEU:HD11   | 1.75                     | 0.64              |
| 13:V:730:GLN:N       | 13:V:731:PRO:CD     | 2.61                     | 0.64              |
| 10:C:1336:ALA:C      | 10:C:1338:ASP:H     | 2.04                     | 0.64              |
| 10:C8:1618:SER:C     | 10:C8:1620:ILE:N    | 2.56                     | 0.64              |
| 11:A32:33:LEU:CD2    | 22:I24:286:LEU:HD13 | 2.27                     | 0.64              |
| 11:A32:706:SER:CB    | 24:D32:1398:ARG:CG  | 2.75                     | 0.64              |
| 18:B:460:PRO:C       | 18:B:562:ARG:HH12   | 1.99                     | 0.64              |
| 18:B:466:PHE:CZ      | 18:B:470:LEU:HD11   | 2.33                     | 0.64              |
| 18:B:1161:LEU:HD11   | 18:B:1403:ILE:CB    | 2.28                     | 0.64              |
| 21:H:154:VAL:HG13    | 21:H:188:ARG:HG2    | 1.80                     | 0.64              |
| 22:I24:298:ALA:HB1   | 22:I24:303:SER:OG   | 1.97                     | 0.64              |
| 24:D40:280:VAL:HG21  | 24:D40:373:PRO:HG2  | 1.78                     | 0.64              |
| 2:M16:257:VAL:HG23   | 2:M16:274:VAL:HG21  | 1.78                     | 0.64              |
| 3:N16:267:TRP:CH2    | 3:N16:294:TRP:CH2   | 2.86                     | 0.64              |
| 7:Q:325:GLU:OE1      | 7:Q:328:ALA:HB2     | 1.97                     | 0.64              |
| 5:P8:10:GLY:HA2      | 5:P8:26:TYR:CE1     | 2.33                     | 0.64              |
| 6:O8:291:SER:HB2     | 6:O8:293:MET:HE2    | 1.78                     | 0.64              |
| 5:P16:101:LEU:HD23   | 5:P16:133:TYR:CZ    | 2.04                     | 0.64              |
| 7:Q16:241:HIS:CD2    | 7:Q16:258:ARG:CZ    | 2.81                     | 0.64              |
| 7:Q16:272:SER:C      | 7:Q16:274:ASN:H     | 2.05                     | 0.64              |
| 10:C16:557:VAL:HG22  | 10:C16:565:ARG:CZ   | 2.26                     | 0.64              |
| 10:C16:865:ASN:OD1   | 10:C16:917:LYS:NZ   | 2.31                     | 0.64              |
| 10:C16:1133:ILE:HG12 | 10:C16:1152:LYS:HD2 | 1.79                     | 0.64              |
| 10:C16:1621:LYS:O    | 10:C16:1622:SER:C   | 2.35                     | 0.64              |
| 10:C24:572:ILE:CG1   | 10:C24:606:MET:HE1  | 2.26                     | 0.64              |
| 10:C24:1548:ILE:HD12 | 24:D24:1407:PHE:HZ  | 1.57                     | 0.64              |
| 10:C24:1814:LYS:NZ   | 23:J24:738:MET:CG   | 2.59                     | 0.64              |
| 11:A40:747:MET:HE1   | 24:D32:167:ARG:HH12 | 1.61                     | 0.64              |
| 14:W:695:LEU:HG      | 15:J:617:LEU:HD11   | 1.78                     | 0.64              |
| 10:C:249:THR:O       | 10:C:251:GLY:N      | 2.30                     | 0.64              |
| 10:C:275:ALA:HB1     | 10:C:326:LEU:CD1    | 2.28                     | 0.64              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C:1339:VAL:HG13   | 10:C:1742:CYS:HB3   | 1.80                     | 0.64              |
| 10:C8:593:ARG:HH12   | 10:C8:655:SER:HG    | 1.41                     | 0.64              |
| 10:C8:847:ARG:NH2    | 10:C8:910:SER:CB    | 2.59                     | 0.64              |
| 10:C8:1230:TYR:CE2   | 10:C8:1295:ALA:HB1  | 2.33                     | 0.64              |
| 11:A16:714:GLY:HA2   | 24:D16:1398:ARG:CZ  | 2.27                     | 0.64              |
| 11:A32:698:LYS:HD3   | 11:A32:804:TYR:CE1  | 2.31                     | 0.64              |
| 18:B8:187:LEU:CD2    | 18:B8:251:PHE:HE2   | 2.11                     | 0.64              |
| 19:4:281:TRP:CE3     | 19:4:288:SER:HB3    | 2.32                     | 0.64              |
| 20:E:353:ILE:CD1     | 20:E:413:PHE:CB     | 2.75                     | 0.64              |
| 20:E8:355:PRO:CA     | 20:E8:454:MET:CE    | 2.68                     | 0.64              |
| 21:H16:316:ILE:O     | 21:H16:316:ILE:HG22 | 1.98                     | 0.64              |
| 10:C32:962:PHE:CE2   | 10:C32:997:ILE:HD13 | 2.33                     | 0.64              |
| 10:C32:1133:ILE:HG12 | 10:C32:1152:LYS:HD2 | 1.79                     | 0.64              |
| 10:C32:1618:SER:C    | 10:C32:1620:ILE:H   | 2.06                     | 0.64              |
| 10:C32:1626:GLN:NE2  | 10:C32:1692:LYS:HZ3 | 1.90                     | 0.64              |
| 2:M8:166:THR:H       | 2:M8:169:THR:HG1    | 1.45                     | 0.64              |
| 2:M16:593:HIS:HD2    | 3:N16:224:LEU:CD2   | 2.10                     | 0.64              |
| 5:P:267:ARG:NH2      | 5:P:270:GLU:CD      | 2.45                     | 0.64              |
| 6:O:119:ARG:HG2      | 6:O:181:GLU:HB3     | 1.79                     | 0.64              |
| 5:P16:402:LEU:HD11   | 5:P16:433:LEU:HD22  | 1.80                     | 0.64              |
| 6:O16:119:ARG:HG2    | 6:O16:181:GLU:HB3   | 1.79                     | 0.64              |
| 8:L8:608:PHE:CG      | 8:L8:635:MET:HG2    | 2.33                     | 0.64              |
| 10:C16:182:ASP:HB2   | 10:C16:183:PRO:CD   | 2.23                     | 0.64              |
| 10:C16:386:ASN:C     | 10:C16:390:HIS:HD1  | 2.01                     | 0.64              |
| 10:C16:1220:SER:O    | 10:C16:1225:ARG:NH2 | 2.31                     | 0.64              |
| 10:C16:1439:ILE:CD1  | 10:C16:1457:LEU:CD1 | 2.75                     | 0.64              |
| 10:C24:1010:ALA:CB   | 10:C24:1192:ARG:NH2 | 2.61                     | 0.64              |
| 10:C24:1111:SER:C    | 10:C24:1113:LYS:H   | 2.05                     | 0.64              |
| 11:A40:43:LEU:HD23   | 23:J16:700:LEU:CD2  | 2.27                     | 0.64              |
| 10:C:390:HIS:HB3     | 10:C:452:LEU:CB     | 2.27                     | 0.64              |
| 10:C:578:LEU:HB3     | 10:C:584:ILE:CD1    | 2.27                     | 0.64              |
| 10:C:1055:GLU:O      | 10:C:1057:THR:N     | 2.30                     | 0.64              |
| 10:C:1618:SER:C      | 10:C:1620:ILE:N     | 2.56                     | 0.64              |
| 10:C:1716:LYS:HG3    | 10:C:1721:GLN:HE21  | 1.61                     | 0.64              |
| 10:C8:847:ARG:CZ     | 10:C8:911:ILE:N     | 2.57                     | 0.64              |
| 10:C8:1010:ALA:HB2   | 10:C8:1192:ARG:NH2  | 2.13                     | 0.64              |
| 10:C8:1339:VAL:HG13  | 10:C8:1742:CYS:HB3  | 1.79                     | 0.64              |
| 18:B:1112:LYS:NZ     | 21:H:327:SER:O      | 2.29                     | 0.64              |
| 18:B8:771:MET:HE3    | 18:B8:840:VAL:HG21  | 1.79                     | 0.64              |
| 18:B8:816:LEU:CD2    | 18:B8:822:ILE:HD13  | 2.28                     | 0.64              |
| 19:4:189:LEU:CB      | 19:4:203:LEU:HD23   | 2.27                     | 0.64              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:743:PHE:CZ    | 10:C32:749:LEU:HD23  | 2.32                     | 0.64              |
| 10:C32:1121:ILE:HG23 | 10:C32:1133:ILE:CD1  | 2.28                     | 0.64              |
| 10:C32:1336:ALA:C    | 10:C32:1338:ASP:H    | 2.04                     | 0.64              |
| 2:M:593:HIS:HD2      | 3:N:224:LEU:CD2      | 2.10                     | 0.63              |
| 2:M8:343:MET:C       | 2:M8:345:ASP:H       | 2.06                     | 0.63              |
| 2:M16:202:LYS:CE     | 2:M16:206:SER:HG     | 2.11                     | 0.63              |
| 5:P:234:TRP:CZ2      | 5:P:334:THR:HA       | 2.34                     | 0.63              |
| 5:P8:50:ARG:NH1      | 6:O8:17:TRP:CE3      | 2.67                     | 0.63              |
| 5:P16:620:ILE:HG21   | 5:P16:660:ARG:NH2    | 2.12                     | 0.63              |
| 10:C16:904:ILE:HD11  | 10:C16:964:LEU:HD12  | 1.80                     | 0.63              |
| 10:C16:1002:LEU:HD12 | 10:C16:1019:ARG:HH12 | 1.61                     | 0.63              |
| 10:C16:1121:ILE:HG23 | 10:C16:1133:ILE:CD1  | 2.28                     | 0.63              |
| 11:A24:33:LEU:CD2    | 22:I8:286:LEU:HD13   | 2.27                     | 0.63              |
| 10:C24:865:ASN:OD1   | 10:C24:917:LYS:NZ    | 2.31                     | 0.63              |
| 10:C24:962:PHE:CE2   | 10:C24:997:ILE:HD13  | 2.33                     | 0.63              |
| 10:C24:1055:GLU:O    | 10:C24:1057:THR:N    | 2.30                     | 0.63              |
| 10:C:1220:SER:O      | 10:C:1225:ARG:NH2    | 2.31                     | 0.63              |
| 10:C:1618:SER:C      | 10:C:1620:ILE:H      | 2.06                     | 0.63              |
| 10:C8:1424:GLN:HE21  | 10:C8:1478:VAL:CG1   | 2.10                     | 0.63              |
| 11:A16:33:LEU:CD2    | 22:I:286:LEU:HD13    | 2.27                     | 0.63              |
| 18:B:1112:LYS:HE3    | 21:H:327:SER:CB      | 2.27                     | 0.63              |
| 18:B8:235:ARG:NH1    | 18:B8:308:GLU:HB3    | 2.13                     | 0.63              |
| 18:B8:671:MET:HE1    | 18:B8:736:ALA:CB     | 2.27                     | 0.63              |
| 18:B8:1121:ALA:O     | 18:B8:1122:SER:C     | 2.35                     | 0.63              |
| 20:E:85:LEU:O        | 20:E:89:LEU:CD1      | 2.46                     | 0.63              |
| 19:48:178:ASN:OD1    | 20:E8:416:LYS:CE     | 2.47                     | 0.63              |
| 19:48:186:GLY:O      | 19:48:187:SER:C      | 2.40                     | 0.63              |
| 22:I8:199:PHE:CE1    | 23:J8:620:MET:HG3    | 2.31                     | 0.63              |
| 22:I8:289:LEU:HD23   | 22:I8:296:ARG:NH2    | 2.10                     | 0.63              |
| 21:H16:139:ASP:OD1   | 21:H16:140:PRO:CD    | 2.34                     | 0.63              |
| 10:C32:1010:ALA:HB2  | 10:C32:1192:ARG:NH2  | 2.14                     | 0.63              |
| 1:R:1101:ARG:CD      | 24:D:1459:LEU:O      | 2.46                     | 0.63              |
| 2:M8:593:HIS:HD2     | 3:N8:224:LEU:CD2     | 2.10                     | 0.63              |
| 2:M16:202:LYS:HE3    | 2:M16:206:SER:HG     | 1.63                     | 0.63              |
| 7:Q:295:SER:CB       | 7:Q:297:VAL:HG23     | 2.27                     | 0.63              |
| 5:P16:206:SER:HG     | 5:P16:207:HIS:CE1    | 2.15                     | 0.63              |
| 6:O16:133:LEU:HD22   | 6:O16:189:LEU:CD2    | 2.29                     | 0.63              |
| 8:L:1064:ASP:OD2     | 9:K:1101:GLU:OE1     | 2.16                     | 0.63              |
| 9:K8:716:ALA:CB      | 10:C32:503:THR:CB    | 2.64                     | 0.63              |
| 10:C16:909:PRO:HB3   | 10:C16:920:LEU:HD22  | 1.80                     | 0.63              |
| 10:C16:1010:ALA:CB   | 10:C16:1192:ARG:NH2  | 2.61                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C16:1618:SER:C   | 10:C16:1620:ILE:N   | 2.56                     | 0.63              |
| 10:C24:1061:ASN:O   | 10:C24:1062:GLU:C   | 2.25                     | 0.63              |
| 10:C24:1618:SER:C   | 10:C24:1620:ILE:N   | 2.56                     | 0.63              |
| 11:A40:501:PRO:HB2  | 11:A40:524:GLU:OE1  | 1.99                     | 0.63              |
| 11:A32:43:LEU:HD23  | 23:J24:700:LEU:CD2  | 2.27                     | 0.63              |
| 11:A32:845:THR:CB   | 24:D32:1297:HIS:CE1 | 2.81                     | 0.63              |
| 18:B:1156:GLN:C     | 18:B:1382:LYS:HZ3   | 2.05                     | 0.63              |
| 18:B8:268:GLN:HE22  | 18:B8:323:GLU:CB    | 2.11                     | 0.63              |
| 18:B8:917:PHE:HE2   | 18:B8:960:GLN:CD    | 2.05                     | 0.63              |
| 18:B8:1618:HIS:ND1  | 18:B8:1622:ILE:HD11 | 2.10                     | 0.63              |
| 18:B8:1839:GLU:O    | 18:B8:1843:THR:OG1  | 2.15                     | 0.63              |
| 20:E8:165:ARG:HH11  | 20:E8:173:ILE:HD11  | 1.62                     | 0.63              |
| 21:H:316:ILE:O      | 21:H:317:ALA:C      | 2.35                     | 0.63              |
| 21:H16:154:VAL:HG13 | 21:H16:188:ARG:HG2  | 1.80                     | 0.63              |
| 23:J16:718:GLN:O    | 23:J16:722:LEU:HD12 | 1.98                     | 0.63              |
| 24:D:308:ASN:HB2    | 24:D16:753:ARG:NH2  | 2.13                     | 0.63              |
| 10:C32:1271:PHE:HE2 | 10:C32:1284:ASP:CB  | 2.06                     | 0.63              |
| 10:C32:1618:SER:C   | 10:C32:1620:ILE:N   | 2.56                     | 0.63              |
| 12:A48:388:VAL:HG23 | 12:A48:459:ARG:NH1  | 2.12                     | 0.63              |
| 1:R:1033:LYS:HZ3    | 24:D:1432:THR:CB    | 2.08                     | 0.63              |
| 2:M:346:VAL:C       | 2:M:348:GLU:N       | 2.56                     | 0.63              |
| 2:M8:346:VAL:C      | 2:M8:348:GLU:N      | 2.56                     | 0.63              |
| 2:M8:851:LEU:HD22   | 4:T8:653:GLN:HE21   | 1.62                     | 0.63              |
| 2:M16:231:ARG:HG3   | 2:M16:299:GLY:HA3   | 1.74                     | 0.63              |
| 2:M16:343:MET:C     | 2:M16:345:ASP:H     | 2.06                     | 0.63              |
| 2:M16:343:MET:C     | 2:M16:345:ASP:N     | 2.56                     | 0.63              |
| 2:M16:503:TYR:CE1   | 2:M16:507:LEU:HD12  | 2.33                     | 0.63              |
| 2:M16:763:ASP:OD1   | 2:M16:818:THR:HG23  | 1.98                     | 0.63              |
| 5:P8:234:TRP:CZ2    | 5:P8:334:THR:HA     | 2.34                     | 0.63              |
| 6:O16:9:ASP:OD2     | 6:O16:51:LYS:HE2    | 1.97                     | 0.63              |
| 8:L8:1058:ILE:HG23  | 9:K8:1083:ILE:CD1   | 2.28                     | 0.63              |
| 8:L16:856:LEU:CD2   | 9:K16:1281:SER:HB2  | 2.28                     | 0.63              |
| 10:C16:717:GLU:CG   | 23:J8:656:ARG:NE    | 2.61                     | 0.63              |
| 10:C16:1358:ASP:O   | 10:C16:1361:LYS:N   | 2.31                     | 0.63              |
| 11:A24:81:LEU:HD21  | 22:I8:309:SER:HA    | 1.80                     | 0.63              |
| 11:A24:501:PRO:HB2  | 11:A24:524:GLU:OE1  | 1.99                     | 0.63              |
| 11:A24:638:LEU:HD21 | 11:A24:663:LEU:HD21 | 1.80                     | 0.63              |
| 10:C24:1230:TYR:CE2 | 10:C24:1295:ALA:HB1 | 2.33                     | 0.63              |
| 10:C24:1618:SER:C   | 10:C24:1620:ILE:H   | 2.06                     | 0.63              |
| 11:A40:312:LEU:HD13 | 11:A40:364:ILE:HD11 | 1.81                     | 0.63              |
| 12:A:312:LEU:HD13   | 12:A:364:ILE:HD11   | 1.81                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A:388:VAL:CG2    | 12:A:459:ARG:HH12   | 2.09                     | 0.63              |
| 11:A16:711:ARG:HD3  | 24:D16:1398:ARG:HG3 | 1.80                     | 0.63              |
| 11:A32:10:TRP:CZ3   | 23:J24:692:VAL:HG22 | 2.34                     | 0.63              |
| 18:B8:460:PRO:C     | 18:B8:562:ARG:HH12  | 1.99                     | 0.63              |
| 24:D8:280:VAL:HG21  | 24:D8:373:PRO:HG2   | 1.78                     | 0.63              |
| 12:A48:388:VAL:CG2  | 12:A48:459:ARG:HH12 | 2.09                     | 0.63              |
| 12:A48:440:LEU:HD12 | 12:A48:443:LEU:HD11 | 1.75                     | 0.63              |
| 12:A48:501:PRO:HB2  | 12:A48:524:GLU:OE1  | 1.99                     | 0.63              |
| 2:M16:628:LEU:HD12  | 3:N16:223:GLY:CA    | 2.19                     | 0.63              |
| 5:P:50:ARG:NH1      | 6:O:17:TRP:CE3      | 2.67                     | 0.63              |
| 5:P8:175:MET:HE2    | 5:P8:433:LEU:HD23   | 1.79                     | 0.63              |
| 6:O8:23:ARG:NE      | 6:O8:37:GLU:OE1     | 2.32                     | 0.63              |
| 6:O8:90:GLU:CD      | 6:O8:98:LYS:HZ2     | 2.06                     | 0.63              |
| 5:P16:143:ASN:HB3   | 5:P16:163:GLU:OE2   | 1.99                     | 0.63              |
| 8:L:1092:LEU:CD1    | 9:K:999:PHE:HD2     | 2.11                     | 0.63              |
| 8:L8:976:LEU:HD21   | 9:K8:1004:ARG:NE    | 2.07                     | 0.63              |
| 8:L16:851:PRO:HB3   | 9:K16:1283:PRO:HB2  | 1.80                     | 0.63              |
| 9:K8:1048:GLN:HE22  | 9:K8:1128:ARG:HG2   | 1.64                     | 0.63              |
| 10:C16:1111:SER:C   | 10:C16:1113:LYS:H   | 2.05                     | 0.63              |
| 10:C16:1265:ARG:C   | 10:C16:1268:ARG:HG2 | 2.19                     | 0.63              |
| 10:C24:275:ALA:HB1  | 10:C24:326:LEU:CD1  | 2.28                     | 0.63              |
| 10:C24:754:MET:HE2  | 10:C24:819:GLN:HB3  | 1.80                     | 0.63              |
| 10:C24:1212:GLU:OE1 | 11:A40:109:HIS:NE2  | 2.26                     | 0.63              |
| 10:C24:1220:SER:O   | 10:C24:1225:ARG:NH2 | 2.31                     | 0.63              |
| 10:C:450:PRO:C      | 10:C:452:LEU:H      | 2.07                     | 0.63              |
| 10:C:667:ILE:HG12   | 10:C:670:GLU:N      | 2.14                     | 0.63              |
| 10:C:1010:ALA:CB    | 10:C:1192:ARG:NH2   | 2.61                     | 0.63              |
| 10:C8:300:VAL:HG12  | 10:C8:317:ARG:CG    | 2.27                     | 0.63              |
| 10:C8:865:ASN:OD1   | 10:C8:917:LYS:NZ    | 2.31                     | 0.63              |
| 10:C8:1439:ILE:CD1  | 10:C8:1457:LEU:CD1  | 2.75                     | 0.63              |
| 11:A32:312:LEU:HD13 | 11:A32:364:ILE:HD11 | 1.81                     | 0.63              |
| 11:A32:845:THR:CB   | 24:D32:1297:HIS:HE1 | 2.12                     | 0.63              |
| 18:B:187:LEU:CD2    | 18:B:251:PHE:HE2    | 2.11                     | 0.63              |
| 18:B:689:SER:C      | 18:B:691:SER:N      | 2.56                     | 0.63              |
| 18:B8:262:HIS:ND1   | 18:B8:379:LEU:CD2   | 2.54                     | 0.63              |
| 18:B8:991:ASP:O     | 18:B8:993:ALA:N     | 2.30                     | 0.63              |
| 21:H24:316:ILE:O    | 21:H24:316:ILE:HG22 | 1.98                     | 0.63              |
| 10:C32:865:ASN:OD1  | 10:C32:917:LYS:NZ   | 2.31                     | 0.63              |
| 2:M:399:THR:OG1     | 2:M:480:ARG:CZ      | 2.46                     | 0.63              |
| 2:M8:188:ARG:HB2    | 3:N8:264:ARG:HH11   | 1.62                     | 0.63              |
| 2:M8:773:VAL:HG13   | 2:M8:829:ALA:HA     | 1.80                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M16:625:HIS:ND1   | 3:N16:165:GLY:CA    | 2.62                     | 0.63              |
| 5:P16:50:ARG:NH1    | 6:O16:17:TRP:CE3    | 2.67                     | 0.63              |
| 5:P16:247:GLU:OE1   | 5:P16:296:PHE:N     | 2.29                     | 0.63              |
| 9:K16:950:LYS:HE2   | 9:K16:974:LEU:CD2   | 2.29                     | 0.63              |
| 10:C16:249:THR:O    | 10:C16:251:GLY:N    | 2.30                     | 0.63              |
| 10:C16:754:MET:HE2  | 10:C16:819:GLN:HB3  | 1.80                     | 0.63              |
| 10:C24:909:PRO:HB3  | 10:C24:920:LEU:HD22 | 1.80                     | 0.63              |
| 11:A40:81:LEU:HD21  | 22:I16:309:SER:HA   | 1.80                     | 0.63              |
| 10:C:667:ILE:CG2    | 10:C:670:GLU:N      | 2.59                     | 0.63              |
| 10:C:1121:ILE:HG23  | 10:C:1133:ILE:CD1   | 2.29                     | 0.63              |
| 10:C8:1618:SER:C    | 10:C8:1620:ILE:H    | 2.06                     | 0.63              |
| 11:A32:154:ILE:HG23 | 18:B8:1851:VAL:CG2  | 2.28                     | 0.63              |
| 18:B:655:SER:OG     | 18:B:658:SER:OG     | 2.14                     | 0.63              |
| 20:E:165:ARG:HH11   | 20:E:173:ILE:HD11   | 1.62                     | 0.63              |
| 19:48:111:LYS:HD2   | 19:48:129:GLU:OE2   | 1.99                     | 0.63              |
| 19:48:251:ARG:O     | 19:48:252:ARG:NH1   | 2.29                     | 0.63              |
| 10:C32:453:LEU:HB3  | 10:C32:486:LEU:CD2  | 2.28                     | 0.63              |
| 1:R:765:ASP:OD1     | 24:D:1361:ALA:CB    | 2.43                     | 0.63              |
| 2:M:810:LEU:HD22    | 2:M:819:GLN:HB3     | 1.81                     | 0.63              |
| 2:M8:627:TYR:OH     | 3:N8:162:THR:HB     | 1.98                     | 0.63              |
| 3:N8:162:THR:HG22   | 3:N8:168:VAL:HG22   | 1.75                     | 0.63              |
| 2:M16:358:LEU:HB2   | 2:M16:359:PRO:HD3   | 1.81                     | 0.63              |
| 6:O8:119:ARG:HG2    | 6:O8:181:GLU:HB3    | 1.79                     | 0.63              |
| 7:Q8:325:GLU:OE1    | 7:Q8:328:ALA:HB2    | 1.97                     | 0.63              |
| 5:P16:547:PHE:CZ    | 7:Q16:227:SER:O     | 2.51                     | 0.63              |
| 8:L8:605:MET:SD     | 8:L8:631:LEU:HD11   | 2.34                     | 0.63              |
| 9:K:1019:ARG:CG     | 9:K:1059:ARG:NH1    | 2.62                     | 0.63              |
| 10:C16:847:ARG:HD2  | 10:C16:911:ILE:HD12 | 1.77                     | 0.63              |
| 10:C24:139:ARG:NE   | 10:C24:380:ASP:OD2  | 2.32                     | 0.63              |
| 10:C24:453:LEU:CB   | 10:C24:486:LEU:HD21 | 2.29                     | 0.63              |
| 10:C:865:ASN:OD1    | 10:C:917:LYS:NZ     | 2.31                     | 0.63              |
| 10:C8:450:PRO:C     | 10:C8:452:LEU:H     | 2.07                     | 0.63              |
| 11:A32:11:THR:CG2   | 22:I24:162:GLN:HE21 | 2.11                     | 0.63              |
| 11:A32:81:LEU:HD21  | 22:I24:309:SER:HA   | 1.80                     | 0.63              |
| 18:B8:395:ARG:HB2   | 18:B8:426:VAL:HG11  | 1.80                     | 0.63              |
| 18:B8:1045:LYS:NZ   | 18:B8:1100:LEU:HD21 | 2.11                     | 0.63              |
| 12:A48:312:LEU:HD13 | 12:A48:364:ILE:HD11 | 1.81                     | 0.63              |
| 2:M:217:ILE:CD1     | 3:N:28:THR:HG21     | 2.29                     | 0.63              |
| 1:R8:1266:THR:N     | 5:P8:684:ARG:NH2    | 2.46                     | 0.63              |
| 2:M8:202:LYS:HE3    | 2:M8:206:SER:HG     | 1.62                     | 0.63              |
| 2:M8:414:GLY:HA2    | 8:L8:401:LYS:HZ3    | 1.62                     | 0.63              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:810:LEU:HD22    | 2:M8:819:GLN:HB3     | 1.81                     | 0.63              |
| 2:M16:217:ILE:CD1    | 3:N16:28:THR:HG21    | 2.29                     | 0.63              |
| 7:Q8:272:SER:C       | 7:Q8:274:ASN:H       | 2.05                     | 0.63              |
| 10:C16:390:HIS:CD2   | 10:C16:449:GLU:HB2   | 2.32                     | 0.63              |
| 10:C16:1286:MET:CE   | 10:C16:1344:VAL:HG11 | 2.29                     | 0.63              |
| 10:C16:1777:SER:O    | 10:C16:1778:ASN:C    | 2.26                     | 0.63              |
| 10:C24:1265:ARG:C    | 10:C24:1268:ARG:HG2  | 2.19                     | 0.63              |
| 10:C24:1688:ARG:HG3  | 23:J24:735:LYS:NZ    | 2.13                     | 0.63              |
| 11:A40:10:TRP:CZ3    | 23:J16:692:VAL:HG22  | 2.34                     | 0.63              |
| 12:A:501:PRO:HB2     | 12:A:524:GLU:OE1     | 1.99                     | 0.63              |
| 14:W:711:ARG:CB      | 10:C8:1609:ASP:OD2   | 2.46                     | 0.63              |
| 10:C:453:LEU:CB      | 10:C:486:LEU:HD21    | 2.29                     | 0.63              |
| 10:C:904:ILE:HD11    | 10:C:964:LEU:HD12    | 1.80                     | 0.63              |
| 10:C8:249:THR:O      | 10:C8:251:GLY:N      | 2.30                     | 0.63              |
| 10:C8:639:MET:CE     | 10:C8:643:LEU:HD11   | 2.28                     | 0.63              |
| 10:C8:904:ILE:HD11   | 10:C8:964:LEU:HD12   | 1.80                     | 0.63              |
| 10:C8:991:LEU:HD11   | 10:C8:1046:SER:OG    | 1.99                     | 0.63              |
| 10:C8:1286:MET:CE    | 10:C8:1344:VAL:HG11  | 2.29                     | 0.63              |
| 11:A16:10:TRP:CZ3    | 23:J32:692:VAL:HG22  | 2.34                     | 0.63              |
| 11:A16:81:LEU:HD21   | 22:I:309:SER:HA      | 1.80                     | 0.63              |
| 18:B:863:MET:HE3     | 18:B:900:LEU:HD21    | 1.81                     | 0.63              |
| 18:B:904:ALA:CB      | 18:B:917:PHE:CZ      | 2.81                     | 0.63              |
| 18:B8:466:PHE:CZ     | 18:B8:470:LEU:HD11   | 2.33                     | 0.63              |
| 19:4:362:ALA:CB      | 19:4:417:ASP:OD2     | 2.46                     | 0.63              |
| 22:I24:196:VAL:HA    | 23:J24:620:MET:HE1   | 0.69                     | 0.63              |
| 10:C32:647:GLU:OE2   | 10:C32:656:THR:OG1   | 2.13                     | 0.63              |
| 2:M:202:LYS:HE3      | 2:M:206:SER:HG       | 1.63                     | 0.63              |
| 2:M:773:VAL:HG13     | 2:M:829:ALA:HA       | 1.80                     | 0.63              |
| 2:M8:399:THR:OG1     | 2:M8:480:ARG:CZ      | 2.47                     | 0.63              |
| 1:R16:1449:TRP:HH2   | 2:M16:161:ASP:C      | 2.06                     | 0.63              |
| 2:M16:417:ARG:CD     | 8:L16:298:PHE:CE2    | 2.81                     | 0.63              |
| 5:P8:55:ARG:NH1      | 5:P8:64:ASP:HB3      | 2.14                     | 0.63              |
| 5:P8:143:ASN:HB3     | 5:P8:163:GLU:OE2     | 1.99                     | 0.63              |
| 6:O8:103:MET:HE1     | 6:O8:124:MET:CE      | 2.28                     | 0.63              |
| 5:P16:234:TRP:CZ2    | 5:P16:334:THR:HA     | 2.34                     | 0.63              |
| 9:K8:955:TYR:CD1     | 9:K8:985:PHE:CD2     | 2.86                     | 0.63              |
| 10:C16:453:LEU:CB    | 10:C16:486:LEU:HD21  | 2.29                     | 0.63              |
| 10:C16:1121:ILE:CG2  | 10:C16:1133:ILE:CD1  | 2.77                     | 0.63              |
| 10:C16:1339:VAL:HG13 | 10:C16:1742:CYS:HB3  | 1.80                     | 0.63              |
| 10:C16:1424:GLN:HE21 | 10:C16:1478:VAL:CG1  | 2.09                     | 0.63              |
| 10:C24:1121:ILE:HG23 | 10:C24:1133:ILE:CD1  | 2.29                     | 0.63              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 13:V:909:ALA:CB      | 14:W:787:MET:HE2    | 2.29                     | 0.63              |
| 14:W:709:LEU:HD11    | 15:J:643:THR:HB     | 1.80                     | 0.63              |
| 15:J:680:LEU:HD23    | 15:J:686:MET:CE     | 2.29                     | 0.63              |
| 10:C:847:ARG:NH2     | 10:C:910:SER:CB     | 2.59                     | 0.63              |
| 10:C:909:PRO:HB3     | 10:C:920:LEU:HD22   | 1.80                     | 0.63              |
| 10:C8:1010:ALA:CB    | 10:C8:1192:ARG:NH2  | 2.61                     | 0.63              |
| 11:A16:11:THR:CG2    | 22:I:162:GLN:HE21   | 2.11                     | 0.63              |
| 11:A16:43:LEU:HD23   | 23:J32:700:LEU:CD2  | 2.27                     | 0.63              |
| 11:A32:437:LEU:HD11  | 11:A32:454:LYS:HE2  | 1.81                     | 0.63              |
| 18:B:266:ARG:NH1     | 18:B:383:PHE:CD1    | 2.67                     | 0.63              |
| 18:B:514:THR:HG22    | 18:B:549:TRP:HH2    | 1.58                     | 0.63              |
| 18:B8:689:SER:C      | 18:B8:691:SER:N     | 2.56                     | 0.63              |
| 18:B8:863:MET:HE3    | 18:B8:900:LEU:HD21  | 1.81                     | 0.63              |
| 18:B8:904:ALA:CB     | 18:B8:917:PHE:CZ    | 2.81                     | 0.63              |
| 19:4:220:TRP:CH2     | 19:4:242:VAL:HG21   | 2.34                     | 0.63              |
| 21:H:200:LEU:HD22    | 23:J32:568:ILE:HD12 | 1.81                     | 0.63              |
| 2:M:417:ARG:CG       | 8:L:346:TRP:CH2     | 2.80                     | 0.63              |
| 2:M:755:THR:HB       | 2:M:757:VAL:HG23    | 1.79                     | 0.63              |
| 1:R8:765:ASP:OD1     | 24:D40:1361:ALA:HB1 | 1.98                     | 0.63              |
| 2:M8:669:ALA:CB      | 2:M8:684:GLN:HG2    | 2.13                     | 0.63              |
| 4:T:669:PRO:HG2      | 5:P:702:LEU:HD13    | 1.79                     | 0.63              |
| 9:K8:730:SER:OG      | 9:K8:735:ASP:OD1    | 2.17                     | 0.63              |
| 11:A24:11:THR:CG2    | 22:I8:162:GLN:HE21  | 2.11                     | 0.63              |
| 11:A24:388:VAL:HG23  | 11:A24:459:ARG:NH1  | 2.12                     | 0.63              |
| 10:C24:1339:VAL:HG13 | 10:C24:1742:CYS:HB3 | 1.80                     | 0.63              |
| 10:C24:1708:ARG:HH21 | 21:H24:275:LYS:CD   | 2.10                     | 0.63              |
| 10:C:1010:ALA:HB2    | 10:C:1192:ARG:NH2   | 2.13                     | 0.63              |
| 10:C8:754:MET:HE2    | 10:C8:819:GLN:HB3   | 1.80                     | 0.63              |
| 11:A16:638:LEU:HD21  | 11:A16:663:LEU:HD21 | 1.80                     | 0.63              |
| 18:B:1205:ILE:HD11   | 18:B:1271:PHE:CE2   | 2.33                     | 0.63              |
| 18:B8:334:PHE:CE1    | 18:B8:338:ILE:HD11  | 2.34                     | 0.63              |
| 19:48:362:ALA:CB     | 19:48:417:ASP:OD2   | 2.46                     | 0.63              |
| 20:E8:447:ILE:HG23   | 20:E8:451:ILE:HG21  | 1.80                     | 0.63              |
| 21:H24:261:ILE:CD1   | 22:I24:195:ALA:HB1  | 2.29                     | 0.63              |
| 24:D40:839:GLU:CB    | 24:D40:971:HIS:CG   | 2.78                     | 0.63              |
| 10:C32:754:MET:HE2   | 10:C32:819:GLN:HB3  | 1.80                     | 0.63              |
| 2:M:503:TYR:CE1      | 2:M:507:LEU:HD12    | 2.33                     | 0.62              |
| 2:M:625:HIS:ND1      | 3:N:165:GLY:CA      | 2.62                     | 0.62              |
| 1:R8:1188:TYR:OH     | 24:D40:1459:LEU:HB3 | 1.99                     | 0.62              |
| 2:M8:625:HIS:ND1     | 3:N8:165:GLY:CA     | 2.62                     | 0.62              |
| 2:M16:346:VAL:C      | 2:M16:348:GLU:N     | 2.56                     | 0.62              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:399:THR:OG1   | 2:M16:480:ARG:CZ     | 2.46                     | 0.62              |
| 5:P:313:TRP:CZ2     | 5:P:345:MET:HE3      | 2.13                     | 0.62              |
| 5:P:467:GLN:HE22    | 6:O:291:SER:CB       | 2.11                     | 0.62              |
| 5:P:510:ILE:HD11    | 7:Q:183:ARG:HH12     | 1.63                     | 0.62              |
| 6:O:133:LEU:HD22    | 6:O:189:LEU:CD2      | 2.29                     | 0.62              |
| 7:Q:241:HIS:CD2     | 7:Q:258:ARG:CZ       | 2.81                     | 0.62              |
| 7:Q16:241:HIS:HA    | 7:Q16:257:LEU:HD12   | 1.79                     | 0.62              |
| 10:C16:105:TRP:O    | 10:C16:932:LYS:O     | 2.17                     | 0.62              |
| 10:C16:345:MET:HE1  | 10:C16:401:ILE:HD13  | 1.41                     | 0.62              |
| 10:C16:1318:ARG:NH2 | 10:C16:1396:SER:CB   | 2.62                     | 0.62              |
| 11:A24:36:ASN:ND2   | 22:I8:293:LYS:HZ1    | 1.97                     | 0.62              |
| 10:C24:847:ARG:HD2  | 10:C24:911:ILE:HD12  | 1.77                     | 0.62              |
| 10:C24:1010:ALA:HB2 | 10:C24:1192:ARG:NH2  | 2.13                     | 0.62              |
| 11:A40:743:ARG:NH2  | 24:D32:699:HIS:CD2   | 2.53                     | 0.62              |
| 10:C:736:ILE:HD11   | 10:C:794:LYS:HZ2     | 1.64                     | 0.62              |
| 10:C8:1693:LYS:NZ   | 10:C8:1749:ASP:OD1   | 2.32                     | 0.62              |
| 11:A16:437:LEU:HD11 | 11:A16:454:LYS:HE2   | 1.81                     | 0.62              |
| 11:A16:493:TYR:OH   | 17:F8:57:PRO:O       | 2.17                     | 0.62              |
| 11:A16:668:HIS:CE1  | 11:A16:672:GLU:OE1   | 2.52                     | 0.62              |
| 19:4:178:ASN:OD1    | 20:E:416:LYS:CE      | 2.47                     | 0.62              |
| 19:48:189:LEU:CB    | 19:48:203:LEU:HD23   | 2.28                     | 0.62              |
| 21:H:312:GLN:NE2    | 22:I:290:ASP:CG      | 2.57                     | 0.62              |
| 21:H:316:ILE:O      | 21:H:316:ILE:HG22    | 1.98                     | 0.62              |
| 22:I:196:VAL:CA     | 23:J32:620:MET:CE    | 2.46                     | 0.62              |
| 21:H8:261:ILE:CD1   | 22:I8:195:ALA:HB1    | 2.29                     | 0.62              |
| 21:H8:316:ILE:O     | 21:H8:316:ILE:HG22   | 1.98                     | 0.62              |
| 22:I8:113:HIS:CG    | 22:I8:114:PRO:HD2    | 2.34                     | 0.62              |
| 21:H16:200:LEU:HD22 | 23:J16:568:ILE:HD12  | 1.81                     | 0.62              |
| 2:M8:342:VAL:CG1    | 2:M8:343:MET:H       | 1.92                     | 0.62              |
| 2:M8:738:ILE:HD11   | 2:M8:779:SER:CB      | 2.29                     | 0.62              |
| 3:N8:267:TRP:HH2    | 3:N8:294:TRP:HH2     | 1.44                     | 0.62              |
| 3:N16:222:LEU:HD11  | 3:N16:270:THR:HA     | 1.82                     | 0.62              |
| 5:P:143:ASN:HB3     | 5:P:163:GLU:OE2      | 1.99                     | 0.62              |
| 7:Q8:221:TRP:CE3    | 7:Q8:222:PHE:CE2     | 2.87                     | 0.62              |
| 5:P16:55:ARG:NH1    | 5:P16:64:ASP:HB3     | 2.14                     | 0.62              |
| 6:O16:61:LYS:NZ     | 6:O16:112:ASP:CG     | 2.48                     | 0.62              |
| 11:A24:288:HIS:HB2  | 11:A24:354:ARG:HH12  | 1.64                     | 0.62              |
| 10:C24:169:GLN:OE1  | 10:C24:169:GLN:CA    | 2.44                     | 0.62              |
| 10:C24:1286:MET:CE  | 10:C24:1344:VAL:HG11 | 2.29                     | 0.62              |
| 10:C24:1699:LYS:CE  | 23:J24:722:LEU:CD2   | 2.73                     | 0.62              |
| 13:V:842:HIS:CE1    | 13:V:846:LEU:CD1     | 2.82                     | 0.62              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 14:W:642:LEU:HD21    | 15:J:568:ILE:CD1    | 2.29                     | 0.62              |
| 10:C:453:LEU:HB3     | 10:C:486:LEU:CD2    | 2.28                     | 0.62              |
| 10:C:1121:ILE:CG2    | 10:C:1133:ILE:CD1   | 2.77                     | 0.62              |
| 10:C8:453:LEU:HB3    | 10:C8:486:LEU:CD2   | 2.28                     | 0.62              |
| 10:C8:894:VAL:HG13   | 10:C8:960:PHE:CE2   | 2.34                     | 0.62              |
| 10:C8:1111:SER:C     | 10:C8:1113:LYS:H    | 2.05                     | 0.62              |
| 10:C8:1121:ILE:HG23  | 10:C8:1133:ILE:CD1  | 2.28                     | 0.62              |
| 10:C8:1271:PHE:HE2   | 10:C8:1284:ASP:HB3  | 1.53                     | 0.62              |
| 10:C8:1290:HIS:CD2   | 10:C8:1334:MET:HE3  | 2.26                     | 0.62              |
| 11:A16:121:GLN:NE2   | 18:B:1559:ALA:HB1   | 2.13                     | 0.62              |
| 11:A16:302:GLN:HE22  | 11:A16:324:ARG:NH1  | 1.96                     | 0.62              |
| 18:B:1668:PHE:CE2    | 18:B:1731:PHE:HD2   | 2.16                     | 0.62              |
| 22:I:113:HIS:CG      | 22:I:114:PRO:HD2    | 2.34                     | 0.62              |
| 22:I16:113:HIS:CG    | 22:I16:114:PRO:HD2  | 2.34                     | 0.62              |
| 10:C32:1621:LYS:O    | 10:C32:1622:SER:C   | 2.35                     | 0.62              |
| 12:A48:668:HIS:CE1   | 12:A48:672:GLU:OE1  | 2.52                     | 0.62              |
| 2:M8:417:ARG:CG      | 8:L8:298:PHE:CE2    | 2.82                     | 0.62              |
| 5:P8:467:GLN:HE22    | 6:O8:291:SER:CB     | 2.11                     | 0.62              |
| 8:L8:179:VAL:HG22    | 10:C32:1360:GLN:CG  | 2.28                     | 0.62              |
| 9:K:1019:ARG:CG      | 9:K:1059:ARG:HH11   | 2.11                     | 0.62              |
| 9:K8:649:MET:CB      | 9:K8:704:ARG:HH21   | 1.93                     | 0.62              |
| 10:C16:16:LEU:CD2    | 10:C16:139:ARG:HH12 | 2.12                     | 0.62              |
| 10:C16:450:PRO:C     | 10:C16:452:LEU:H    | 2.07                     | 0.62              |
| 10:C16:1010:ALA:HB2  | 10:C16:1192:ARG:NH2 | 2.13                     | 0.62              |
| 10:C24:450:PRO:C     | 10:C24:452:LEU:H    | 2.07                     | 0.62              |
| 10:C24:1278:ASP:O    | 10:C24:1734:ARG:NH1 | 2.32                     | 0.62              |
| 10:C24:1821:VAL:HG11 | 11:A40:144:LYS:HE3  | 1.81                     | 0.62              |
| 14:W:96:LYS:CE       | 14:W:144:VAL:HG21   | 2.28                     | 0.62              |
| 10:C:754:MET:HE2     | 10:C:819:GLN:HB3    | 1.80                     | 0.62              |
| 10:C:991:LEU:HD11    | 10:C:1046:SER:OG    | 1.99                     | 0.62              |
| 11:A32:121:GLN:NE2   | 18:B8:1559:ALA:HB1  | 2.13                     | 0.62              |
| 11:A32:501:PRO:HB2   | 11:A32:524:GLU:OE1  | 1.98                     | 0.62              |
| 18:B:991:ASP:O       | 18:B:993:ALA:N      | 2.30                     | 0.62              |
| 18:B8:750:GLU:HG3    | 18:B8:760:ARG:NE    | 2.14                     | 0.62              |
| 19:48:122:GLN:HG2    | 19:48:140:THR:HG22  | 1.82                     | 0.62              |
| 21:H8:254:MET:HE1    | 22:I8:192:ALA:HB2   | 1.80                     | 0.62              |
| 21:H16:261:ILE:CD1   | 22:I16:195:ALA:HB1  | 2.29                     | 0.62              |
| 10:C32:453:LEU:CB    | 10:C32:486:LEU:HD21 | 2.29                     | 0.62              |
| 10:C32:768:ARG:CZ    | 10:C32:775:LYS:CG   | 2.69                     | 0.62              |
| 10:C32:1821:VAL:HG11 | 12:A48:144:LYS:HE3  | 1.81                     | 0.62              |
| 12:A48:302:GLN:HE21  | 12:A48:324:ARG:NH1  | 1.98                     | 0.62              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R:1330:ALA:HB3    | 10:C:1173:LEU:HD13   | 1.74                     | 0.62              |
| 1:R:1449:TRP:HH2    | 2:M:161:ASP:C        | 2.06                     | 0.62              |
| 2:M8:202:LYS:CE     | 2:M8:206:SER:HG      | 2.11                     | 0.62              |
| 1:R16:1449:TRP:CH2  | 2:M16:160:LEU:CD1    | 2.82                     | 0.62              |
| 2:M16:231:ARG:HG3   | 2:M16:299:GLY:CA     | 2.26                     | 0.62              |
| 2:M16:810:LEU:HD22  | 2:M16:819:GLN:HB3    | 1.81                     | 0.62              |
| 6:O:23:ARG:NE       | 6:O:37:GLU:OE1       | 2.32                     | 0.62              |
| 6:O:103:MET:HE1     | 6:O:124:MET:CE       | 2.28                     | 0.62              |
| 5:P8:30:TYR:HE2     | 5:P8:32:LEU:HB2      | 1.65                     | 0.62              |
| 5:P8:510:ILE:HD11   | 7:Q8:183:ARG:HH12    | 1.63                     | 0.62              |
| 5:P16:607:PHE:HB3   | 5:P16:629:ARG:CZ     | 2.29                     | 0.62              |
| 10:C16:991:LEU:HD11 | 10:C16:1046:SER:OG   | 1.99                     | 0.62              |
| 11:A24:668:HIS:CE1  | 11:A24:672:GLU:OE1   | 2.52                     | 0.62              |
| 10:C24:453:LEU:HB3  | 10:C24:486:LEU:CD2   | 2.28                     | 0.62              |
| 12:A:668:HIS:HE1    | 12:A:672:GLU:OE1     | 1.82                     | 0.62              |
| 13:V:909:ALA:HB2    | 15:J:703:LEU:HD21    | 1.81                     | 0.62              |
| 14:W:659:ARG:HH12   | 15:J:583:LEU:HD21    | 1.63                     | 0.62              |
| 10:C:1286:MET:CE    | 10:C:1344:VAL:HG11   | 2.29                     | 0.62              |
| 18:B:750:GLU:HG3    | 18:B:760:ARG:NH2     | 2.15                     | 0.62              |
| 18:B:1505:MET:HE1   | 18:B:1518:VAL:HG21   | 1.81                     | 0.62              |
| 18:B8:50:THR:HG21   | 18:B8:179:GLN:HE22   | 1.63                     | 0.62              |
| 18:B8:266:ARG:NH1   | 18:B8:383:PHE:CD1    | 2.67                     | 0.62              |
| 18:B8:1505:MET:HE1  | 18:B8:1518:VAL:HG21  | 1.81                     | 0.62              |
| 19:4:180:ALA:CB     | 19:4:202:ILE:HD11    | 2.14                     | 0.62              |
| 21:H24:200:LEU:HD22 | 23:J24:568:ILE:HD12  | 1.81                     | 0.62              |
| 21:H24:254:MET:HE1  | 22:I24:192:ALA:HB2   | 1.80                     | 0.62              |
| 10:C32:139:ARG:NE   | 10:C32:380:ASP:OD2   | 2.32                     | 0.62              |
| 10:C32:909:PRO:HB3  | 10:C32:920:LEU:HD22  | 1.80                     | 0.62              |
| 10:C32:1286:MET:CE  | 10:C32:1344:VAL:HG11 | 2.29                     | 0.62              |
| 10:C32:1661:LEU:O   | 10:C32:1662:ASP:C    | 2.29                     | 0.62              |
| 2:M:343:MET:C       | 2:M:345:ASP:H        | 2.06                     | 0.62              |
| 2:M8:776:LEU:HD23   | 2:M8:795:TYR:CD2     | 2.35                     | 0.62              |
| 7:Q:241:HIS:CD2     | 7:Q:258:ARG:HE       | 2.16                     | 0.62              |
| 5:P16:467:GLN:HE22  | 6:O16:291:SER:CB     | 2.11                     | 0.62              |
| 6:O16:103:MET:HE1   | 6:O16:124:MET:CE     | 2.28                     | 0.62              |
| 8:L16:1081:MET:SD   | 9:K16:1083:ILE:CG2   | 2.88                     | 0.62              |
| 9:K8:734:TRP:CZ2    | 9:K8:738:GLN:NE2     | 2.68                     | 0.62              |
| 9:K8:787:PRO:HG2    | 9:K8:790:THR:OG1     | 1.99                     | 0.62              |
| 10:C16:453:LEU:HB3  | 10:C16:486:LEU:CD2   | 2.28                     | 0.62              |
| 10:C16:578:LEU:HB3  | 10:C16:584:ILE:CD1   | 2.27                     | 0.62              |
| 11:A24:10:TRP:CZ3   | 23:J8:692:VAL:HG22   | 2.34                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A24:437:LEU:HD11 | 11:A24:454:LYS:HE2  | 1.81                     | 0.62              |
| 10:C24:1547:LYS:CE  | 24:D24:1405:GLY:N   | 2.57                     | 0.62              |
| 11:A40:288:HIS:HB2  | 11:A40:354:ARG:HH12 | 1.65                     | 0.62              |
| 12:A:560:MET:CE     | 12:A:615:GLN:CD     | 2.73                     | 0.62              |
| 10:C:139:ARG:NE     | 10:C:380:ASP:OD2    | 2.32                     | 0.62              |
| 10:C:643:LEU:HD11   | 10:C:679:ARG:HH11   | 0.80                     | 0.62              |
| 10:C:1333:HIS:CE1   | 10:C:1337:LEU:HD22  | 2.35                     | 0.62              |
| 10:C8:1594:PRO:HB3  | 10:C8:1645:PHE:CD1  | 2.35                     | 0.62              |
| 11:A32:388:VAL:HG23 | 11:A32:459:ARG:NH1  | 2.12                     | 0.62              |
| 18:B:334:PHE:CE1    | 18:B:338:ILE:HD11   | 2.34                     | 0.62              |
| 18:B:1436:PRO:CB    | 24:D16:1259:SER:O   | 2.33                     | 0.62              |
| 18:B8:1161:LEU:HD11 | 18:B8:1403:ILE:HD12 | 1.77                     | 0.62              |
| 18:B8:1668:PHE:CE2  | 18:B8:1731:PHE:HD2  | 2.16                     | 0.62              |
| 18:B8:1848:VAL:CG1  | 18:B8:1850:TYR:CE1  | 2.83                     | 0.62              |
| 19:4:111:LYS:HD2    | 19:4:129:GLU:OE2    | 1.99                     | 0.62              |
| 19:48:220:TRP:CH2   | 19:48:242:VAL:HG21  | 2.34                     | 0.62              |
| 21:H:291:VAL:HG22   | 22:I:273:LEU:HD21   | 1.81                     | 0.62              |
| 21:H16:254:MET:HE1  | 22:I16:192:ALA:HB2  | 1.80                     | 0.62              |
| 24:D:409:LEU:HD13   | 24:D16:746:ALA:C    | 2.19                     | 0.62              |
| 10:C32:1234:ASP:OD1 | 10:C32:1302:LYS:NZ  | 2.25                     | 0.62              |
| 1:R8:1078:SER:OG    | 5:P8:713:LEU:CD2    | 2.47                     | 0.62              |
| 1:R8:1188:TYR:CE1   | 24:D40:1459:LEU:HB2 | 2.34                     | 0.62              |
| 2:M8:784:GLY:CA     | 8:L16:472:GLU:OE2   | 2.47                     | 0.62              |
| 6:O8:133:LEU:HD22   | 6:O8:189:LEU:CD2    | 2.29                     | 0.62              |
| 5:P16:10:GLY:HA2    | 5:P16:26:TYR:CE1    | 2.33                     | 0.62              |
| 6:O16:23:ARG:NE     | 6:O16:37:GLU:OE1    | 2.32                     | 0.62              |
| 6:O16:90:GLU:CD     | 6:O16:98:LYS:NZ     | 2.58                     | 0.62              |
| 8:L16:976:LEU:HD21  | 9:K16:1004:ARG:HD2  | 1.73                     | 0.62              |
| 9:K:1180:TRP:CG     | 9:K:1261:MET:CE     | 2.83                     | 0.62              |
| 9:K8:792:LEU:CG     | 9:K8:864:ILE:CD1    | 2.76                     | 0.62              |
| 10:C16:62:ILE:CD1   | 10:C16:72:LEU:CD1   | 2.73                     | 0.62              |
| 10:C16:1290:HIS:CB  | 10:C16:1334:MET:CE  | 2.72                     | 0.62              |
| 11:A24:560:MET:CE   | 11:A24:615:GLN:CD   | 2.73                     | 0.62              |
| 10:C24:578:LEU:HB3  | 10:C24:584:ILE:CD1  | 2.27                     | 0.62              |
| 10:C24:991:LEU:HD11 | 10:C24:1046:SER:OG  | 1.99                     | 0.62              |
| 10:C24:1358:ASP:O   | 10:C24:1361:LYS:N   | 2.31                     | 0.62              |
| 10:C:626:GLN:O      | 10:C:627:VAL:C      | 2.38                     | 0.62              |
| 10:C:653:TYR:HH     | 10:C:679:ARG:HB3    | 1.64                     | 0.62              |
| 10:C8:1220:SER:O    | 10:C8:1225:ARG:NH2  | 2.31                     | 0.62              |
| 11:A32:638:LEU:HD21 | 11:A32:663:LEU:HD21 | 1.80                     | 0.62              |
| 18:B:846:SER:HG     | 18:B:899:LYS:NZ     | 1.68                     | 0.62              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:1112:LYS:CE     | 21:H:327:SER:HB3     | 2.29                     | 0.62              |
| 18:B:1528:PRO:HA     | 18:B:1531:TRP:CE2    | 2.34                     | 0.62              |
| 19:48:350:THR:O      | 19:48:374:GLY:HA2    | 2.00                     | 0.62              |
| 21:H8:312:GLN:NE2    | 22:I8:290:ASP:CG     | 2.57                     | 0.62              |
| 22:I16:97:THR:HG22   | 22:I16:107:THR:HG21  | 1.81                     | 0.62              |
| 24:D32:1112:ALA:HB2  | 24:D32:1160:LEU:HD13 | 1.80                     | 0.62              |
| 10:C32:16:LEU:CD2    | 10:C32:139:ARG:HH12  | 2.12                     | 0.62              |
| 10:C32:643:LEU:HD11  | 10:C32:679:ARG:HH11  | 0.80                     | 0.62              |
| 10:C32:1211:VAL:HG13 | 10:C32:1232:ILE:HD13 | 1.82                     | 0.62              |
| 12:A48:212:LYS:HE3   | 12:A48:585:MET:HE1   | 1.27                     | 0.62              |
| 2:M16:627:TYR:CZ     | 3:N16:162:THR:HB     | 2.35                     | 0.62              |
| 5:P:10:GLY:HA2       | 5:P:26:TYR:CE1       | 2.33                     | 0.62              |
| 7:Q:272:SER:C        | 7:Q:274:ASN:N        | 2.58                     | 0.62              |
| 9:K8:894:LYS:CE      | 9:K8:1058:GLU:O      | 2.42                     | 0.62              |
| 9:K8:1180:TRP:CG     | 9:K8:1261:MET:CE     | 2.83                     | 0.62              |
| 10:C16:668:ALA:HA    | 10:C16:700:MET:HE3   | 1.76                     | 0.62              |
| 10:C24:105:TRP:O     | 10:C24:932:LYS:O     | 2.16                     | 0.62              |
| 10:C24:1594:PRO:HB3  | 10:C24:1645:PHE:CD1  | 2.35                     | 0.62              |
| 11:A40:437:LEU:HD11  | 11:A40:454:LYS:HE2   | 1.81                     | 0.62              |
| 14:W:586:ILE:CG1     | 15:J:572:ASP:OD2     | 2.48                     | 0.62              |
| 14:W:722:GLN:NE2     | 10:C8:1497:LYS:O     | 2.32                     | 0.62              |
| 10:C:792:PHE:CD1     | 10:C:850:ARG:NH1     | 2.68                     | 0.62              |
| 10:C:1660:SER:C      | 10:C:1662:ASP:H      | 2.08                     | 0.62              |
| 10:C8:62:ILE:CD1     | 10:C8:72:LEU:CD1     | 2.73                     | 0.62              |
| 10:C8:960:PHE:CZ     | 10:C8:1138:GLU:HG2   | 2.09                     | 0.62              |
| 11:A16:312:LEU:HD13  | 11:A16:364:ILE:HD11  | 1.81                     | 0.62              |
| 18:B:1674:ASP:C      | 18:B:1676:VAL:H      | 2.06                     | 0.62              |
| 18:B8:810:THR:OG1    | 18:B8:879:SER:O      | 2.17                     | 0.62              |
| 19:4:122:GLN:HG2     | 19:4:140:THR:HG22    | 1.82                     | 0.62              |
| 19:4:186:GLY:O       | 19:4:187:SER:C       | 2.40                     | 0.62              |
| 24:D16:1112:ALA:CB   | 24:D16:1160:LEU:HD13 | 2.30                     | 0.62              |
| 24:D40:853:MET:HB3   | 24:D40:925:ASP:OD2   | 2.00                     | 0.62              |
| 10:C32:1121:ILE:CG2  | 10:C32:1133:ILE:CD1  | 2.77                     | 0.62              |
| 1:R:1165:MET:HE3     | 1:R:1220:GLN:HG3     | 1.80                     | 0.62              |
| 2:M:250:LEU:HD23     | 2:M:287:TYR:CD2      | 2.35                     | 0.62              |
| 2:M16:773:VAL:HG13   | 2:M16:829:ALA:HA     | 1.79                     | 0.62              |
| 7:Q16:295:SER:C      | 7:Q16:297:VAL:N      | 2.54                     | 0.62              |
| 8:L8:977:PRO:CD      | 9:K8:1004:ARG:HD2    | 2.28                     | 0.62              |
| 9:K8:577:GLN:HG2     | 9:K8:625:ARG:NH1     | 2.15                     | 0.62              |
| 9:K8:700:MET:CE      | 9:K8:767:LEU:HD13    | 2.30                     | 0.62              |
| 9:K8:1039:ASP:CG     | 9:K8:1096:LYS:HZ1    | 2.08                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C16:1594:PRO:HB3 | 10:C16:1645:PHE:CD1 | 2.35                     | 0.62              |
| 11:A40:302:GLN:HE22 | 11:A40:324:ARG:NH1  | 1.96                     | 0.62              |
| 12:A:668:HIS:CE1    | 12:A:672:GLU:OE1    | 2.52                     | 0.62              |
| 13:V:842:HIS:CE1    | 13:V:846:LEU:HD11   | 2.35                     | 0.62              |
| 10:C:1594:PRO:HB3   | 10:C:1645:PHE:CD1   | 2.35                     | 0.62              |
| 10:C8:16:LEU:CD2    | 10:C8:139:ARG:HH12  | 2.12                     | 0.62              |
| 10:C8:139:ARG:NE    | 10:C8:380:ASP:OD2   | 2.32                     | 0.62              |
| 10:C8:1333:HIS:CE1  | 10:C8:1337:LEU:HD22 | 2.35                     | 0.62              |
| 10:C8:1821:VAL:HG11 | 16:A8:144:LYS:HE3   | 1.81                     | 0.62              |
| 11:A16:90:PHE:HB3   | 18:B:1800:ARG:HH21  | 0.52                     | 0.62              |
| 11:A32:668:HIS:CE1  | 11:A32:672:GLU:OE1  | 2.52                     | 0.62              |
| 18:B:1848:VAL:CG1   | 18:B:1850:TYR:CE1   | 2.83                     | 0.62              |
| 18:B8:712:PRO:HG3   | 18:B8:759:MET:CE    | 2.23                     | 0.62              |
| 18:B8:1377:ASP:OD2  | 18:B8:1381:ARG:NH2  | 2.30                     | 0.62              |
| 19:4:29:ARG:O       | 19:4:33:THR:OG1     | 2.17                     | 0.62              |
| 19:4:352:CYS:SG     | 19:4:371:TYR:HB2    | 2.39                     | 0.62              |
| 21:H8:200:LEU:HD22  | 23:J8:568:ILE:HD12  | 1.81                     | 0.62              |
| 21:H24:291:VAL:HG22 | 22:I24:273:LEU:HD21 | 1.81                     | 0.62              |
| 10:C32:450:PRO:C    | 10:C32:452:LEU:H    | 2.07                     | 0.62              |
| 10:C32:792:PHE:CD1  | 10:C32:850:ARG:NH1  | 2.68                     | 0.62              |
| 10:C32:1050:HIS:CE1 | 10:C32:1086:LYS:HZ1 | 2.14                     | 0.62              |
| 10:C32:1318:ARG:NH2 | 10:C32:1396:SER:CB  | 2.62                     | 0.62              |
| 1:R:1328:LYS:HA     | 10:C:1173:LEU:CD2   | 2.30                     | 0.62              |
| 1:R:1449:TRP:CH2    | 2:M:160:LEU:CD1     | 2.82                     | 0.62              |
| 2:M:755:THR:C       | 2:M:757:VAL:N       | 2.57                     | 0.62              |
| 1:R8:1466:LYS:CD    | 6:O8:160:LEU:HD13   | 2.29                     | 0.62              |
| 3:N8:222:LEU:HD11   | 3:N8:270:THR:HA     | 1.82                     | 0.62              |
| 1:R16:1449:TRP:CH2  | 2:M16:161:ASP:C     | 2.78                     | 0.62              |
| 2:M16:627:TYR:CG    | 3:N16:167:LEU:HA    | 2.35                     | 0.62              |
| 2:M16:755:THR:C     | 2:M16:757:VAL:N     | 2.57                     | 0.62              |
| 5:P:600:PHE:CG      | 5:P:638:SER:CB      | 2.78                     | 0.62              |
| 7:Q:221:TRP:CE3     | 7:Q:222:PHE:CE2     | 2.87                     | 0.62              |
| 8:L8:605:MET:HG2    | 8:L8:631:LEU:HD13   | 1.81                     | 0.62              |
| 8:L16:1068:PHE:O    | 8:L16:1068:PHE:CD1  | 2.50                     | 0.62              |
| 10:C16:139:ARG:NE   | 10:C16:380:ASP:OD2  | 2.32                     | 0.62              |
| 10:C16:1278:ASP:O   | 10:C16:1734:ARG:NH1 | 2.32                     | 0.62              |
| 11:A24:312:LEU:HD13 | 11:A24:364:ILE:HD11 | 1.81                     | 0.62              |
| 11:A24:683:GLN:OE1  | 11:A24:692:ALA:HA   | 2.00                     | 0.62              |
| 10:C24:33:ILE:CG2   | 10:C24:158:LEU:HD22 | 2.30                     | 0.62              |
| 11:A40:11:THR:CG2   | 22:I16:162:GLN:HE21 | 2.11                     | 0.62              |
| 11:A40:638:LEU:HD21 | 11:A40:663:LEU:HD21 | 1.80                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:643:LEU:CD2    | 10:C:675:ASP:CG     | 2.69                     | 0.62              |
| 10:C:1163:LEU:CD2   | 10:C:1166:SER:CB    | 2.74                     | 0.62              |
| 10:C:1278:ASP:O     | 10:C:1734:ARG:NH1   | 2.32                     | 0.62              |
| 10:C8:1358:ASP:O    | 10:C8:1361:LYS:N    | 2.31                     | 0.62              |
| 11:A16:676:TYR:HE2  | 24:D16:1396:PRO:N   | 1.97                     | 0.62              |
| 11:A16:676:TYR:HH   | 24:D16:1394:SER:C   | 2.07                     | 0.62              |
| 20:E:38:PHE:O       | 20:E:39:SER:C       | 2.41                     | 0.62              |
| 21:H:139:ASP:OD1    | 21:H:140:PRO:CD     | 2.34                     | 0.62              |
| 22:I:97:THR:HG22    | 22:I:107:THR:HG21   | 1.81                     | 0.62              |
| 21:H8:154:VAL:HG13  | 21:H8:188:ARG:HG2   | 1.80                     | 0.62              |
| 21:H24:312:GLN:NE2  | 22:I24:290:ASP:CG   | 2.57                     | 0.62              |
| 22:I16:196:VAL:HA   | 23:J16:620:MET:HE1  | 0.69                     | 0.62              |
| 10:C32:904:ILE:HD11 | 10:C32:964:LEU:HD12 | 1.80                     | 0.62              |
| 10:C32:1010:ALA:CB  | 10:C32:1192:ARG:NH2 | 2.62                     | 0.62              |
| 2:M:251:HIS:CE1     | 2:M:273:VAL:HG21    | 2.35                     | 0.62              |
| 2:M:417:ARG:HA      | 8:L:346:TRP:HZ2     | 1.64                     | 0.62              |
| 1:R8:1165:MET:HE3   | 1:R8:1220:GLN:HG3   | 1.80                     | 0.62              |
| 2:M8:251:HIS:CE1    | 2:M8:273:VAL:HG21   | 2.35                     | 0.62              |
| 2:M16:776:LEU:HD23  | 2:M16:795:TYR:CD2   | 2.35                     | 0.62              |
| 5:P:109:ILE:HD11    | 14:W:18:PRO:HG3     | 1.80                     | 0.62              |
| 7:Q:297:VAL:CG2     | 7:Q:318:GLU:OE1     | 2.48                     | 0.62              |
| 6:O8:90:GLU:CD      | 6:O8:98:LYS:NZ      | 2.58                     | 0.62              |
| 7:Q8:254:ALA:CB     | 7:Q8:302:ILE:HD13   | 2.30                     | 0.62              |
| 7:Q8:272:SER:C      | 7:Q8:274:ASN:N      | 2.58                     | 0.62              |
| 8:L8:179:VAL:HG22   | 10:C32:1360:GLN:HG2 | 1.82                     | 0.62              |
| 8:L8:976:LEU:HD21   | 9:K8:1004:ARG:HE    | 1.62                     | 0.62              |
| 9:K8:631:VAL:CG1    | 9:K8:764:VAL:HB     | 2.27                     | 0.62              |
| 9:K8:975:MET:HA     | 9:K8:985:PHE:HE1    | 1.65                     | 0.62              |
| 10:C16:1212:GLU:OE1 | 11:A24:109:HIS:NE2  | 2.26                     | 0.62              |
| 10:C24:1622:SER:OG  | 10:C24:1623:ILE:N   | 2.08                     | 0.62              |
| 11:A40:560:MET:CE   | 11:A40:615:GLN:CD   | 2.73                     | 0.62              |
| 11:A40:668:HIS:CE1  | 11:A40:672:GLU:OE1  | 2.53                     | 0.62              |
| 10:C8:26:ARG:NH2    | 10:C8:148:GLU:OE2   | 2.33                     | 0.62              |
| 10:C8:33:ILE:CG2    | 10:C8:158:LEU:HD22  | 2.30                     | 0.62              |
| 11:A32:137:GLU:CG   | 18:B8:1901:GLN:NE2  | 2.39                     | 0.62              |
| 11:A32:302:GLN:HE22 | 11:A32:324:ARG:NH1  | 1.96                     | 0.62              |
| 18:B8:112:GLU:OE2   | 18:B8:130:MET:CE    | 2.44                     | 0.62              |
| 21:H:254:MET:HE1    | 22:I:192:ALA:HB2    | 1.80                     | 0.62              |
| 22:I:196:VAL:HA     | 23:J32:620:MET:HE1  | 0.69                     | 0.62              |
| 22:I8:97:THR:HG22   | 22:I8:107:THR:HG21  | 1.81                     | 0.62              |
| 22:I24:113:HIS:CG   | 22:I24:114:PRO:HD2  | 2.34                     | 0.62              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D8:1428:ASN:OD1   | 24:D16:968:ILE:HD11  | 2.00                     | 0.62              |
| 2:M8:217:ILE:CD1     | 3:N8:28:THR:HG21     | 2.29                     | 0.61              |
| 2:M16:251:HIS:CE1    | 2:M16:273:VAL:HG21   | 2.35                     | 0.61              |
| 5:P:547:PHE:CZ       | 7:Q:227:SER:O        | 2.51                     | 0.61              |
| 5:P:638:SER:O        | 5:P:640:PRO:HD3      | 2.00                     | 0.61              |
| 6:O8:119:ARG:HH22    | 6:O8:182:GLU:HG2     | 1.59                     | 0.61              |
| 7:Q8:136:ARG:NH1     | 7:Q8:138:GLU:OE2     | 2.33                     | 0.61              |
| 5:P16:30:TYR:HE2     | 5:P16:32:LEU:HB2     | 1.65                     | 0.61              |
| 7:Q16:241:HIS:CD2    | 7:Q16:258:ARG:HE     | 2.16                     | 0.61              |
| 8:L:1069:LEU:HD11    | 9:K:1086:VAL:CG1     | 2.10                     | 0.61              |
| 9:K:1046:LEU:O       | 9:K:1048:GLN:N       | 2.33                     | 0.61              |
| 9:K:1048:GLN:NE2     | 9:K:1128:ARG:CG      | 2.62                     | 0.61              |
| 10:C16:33:ILE:CG2    | 10:C16:158:LEU:HD22  | 2.30                     | 0.61              |
| 10:C16:1211:VAL:HG13 | 10:C16:1232:ILE:HD13 | 1.82                     | 0.61              |
| 11:A24:302:GLN:HE22  | 11:A24:324:ARG:NH1   | 1.96                     | 0.61              |
| 10:C24:26:ARG:NH2    | 10:C24:148:GLU:OE2   | 2.33                     | 0.61              |
| 10:C:1010:ALA:HA     | 10:C:1192:ARG:HH21   | 1.65                     | 0.61              |
| 10:C:1015:SER:OG     | 10:C:1019:ARG:NH1    | 2.33                     | 0.61              |
| 10:C:1358:ASP:O      | 10:C:1361:LYS:N      | 2.31                     | 0.61              |
| 18:B:816:LEU:CD2     | 18:B:822:ILE:HD13    | 2.28                     | 0.61              |
| 18:B8:1548:LEU:HD11  | 18:B8:1564:PHE:CE2   | 2.35                     | 0.61              |
| 20:E8:473:LEU:HD11   | 20:E8:514:PHE:HB3    | 1.82                     | 0.61              |
| 21:H:261:ILE:CD1     | 22:I:195:ALA:HB1     | 2.29                     | 0.61              |
| 21:H:363:MET:SD      | 22:I:332:MET:CE      | 2.81                     | 0.61              |
| 10:C32:991:LEU:HD11  | 10:C32:1046:SER:OG   | 1.99                     | 0.61              |
| 12:A48:302:GLN:HE22  | 12:A48:324:ARG:NH1   | 1.96                     | 0.61              |
| 2:M:254:LEU:HD21     | 2:M:283:ILE:CG1      | 2.26                     | 0.61              |
| 3:N:267:TRP:CH2      | 3:N:294:TRP:CH2      | 2.86                     | 0.61              |
| 4:T:156:SER:O        | 4:T:160:HIS:CE1      | 2.53                     | 0.61              |
| 4:T16:156:SER:O      | 4:T16:160:HIS:CE1    | 2.53                     | 0.61              |
| 5:P:214:LEU:HD23     | 5:P:236:VAL:HG13     | 1.81                     | 0.61              |
| 5:P:375:LYS:HD3      | 14:W:80:ARG:NH1      | 2.15                     | 0.61              |
| 7:Q:236:HIS:CE1      | 7:Q:238:SER:OG       | 2.53                     | 0.61              |
| 5:P8:101:LEU:CD2     | 5:P8:133:TYR:CG      | 2.83                     | 0.61              |
| 5:P8:547:PHE:CZ      | 7:Q8:227:SER:O       | 2.51                     | 0.61              |
| 5:P8:614:VAL:CG2     | 5:P8:629:ARG:NE      | 2.62                     | 0.61              |
| 5:P8:638:SER:O       | 5:P8:640:PRO:HD3     | 2.00                     | 0.61              |
| 7:Q8:297:VAL:CG2     | 7:Q8:318:GLU:OE1     | 2.48                     | 0.61              |
| 5:P16:638:SER:O      | 5:P16:640:PRO:HD3    | 2.00                     | 0.61              |
| 5:P16:663:LEU:HB2    | 5:P16:707:ASN:ND2    | 2.14                     | 0.61              |
| 9:K:700:MET:CE       | 9:K:767:LEU:HD13     | 2.30                     | 0.61              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:734:TRP:CZ2      | 9:K:738:GLN:NE2      | 2.68                     | 0.61              |
| 11:A24:302:GLN:HE21  | 11:A24:324:ARG:NH1   | 1.97                     | 0.61              |
| 10:C24:798:VAL:CG1   | 10:C24:802:TRP:CZ2   | 2.83                     | 0.61              |
| 10:C24:1121:ILE:CG2  | 10:C24:1133:ILE:CD1  | 2.77                     | 0.61              |
| 10:C24:1449:GLU:OE2  | 24:D24:1151:SER:HA   | 2.00                     | 0.61              |
| 12:A:156:MET:HE3     | 10:C8:58:GLN:O       | 1.36                     | 0.61              |
| 10:C:16:LEU:CD2      | 10:C:139:ARG:HH12    | 2.12                     | 0.61              |
| 10:C:1537:GLU:OE2    | 10:C8:113:LEU:CD2    | 2.44                     | 0.61              |
| 10:C8:909:PRO:HB3    | 10:C8:920:LEU:HD22   | 1.80                     | 0.61              |
| 10:C8:1074:LEU:O     | 10:C8:1076:TYR:N     | 2.33                     | 0.61              |
| 18:B8:1674:ASP:C     | 18:B8:1676:VAL:H     | 2.06                     | 0.61              |
| 22:I:203:GLN:HB3     | 22:I:209:TRP:CZ2     | 2.34                     | 0.61              |
| 24:D24:854:GLU:HA    | 24:D24:857:THR:HG22  | 1.82                     | 0.61              |
| 10:C32:296:PHE:CE1   | 10:C32:300:VAL:HG21  | 2.36                     | 0.61              |
| 10:C32:1074:LEU:O    | 10:C32:1076:TYR:N    | 2.33                     | 0.61              |
| 2:M16:672:TYR:CE2    | 2:M16:680:LYS:NZ     | 2.53                     | 0.61              |
| 5:P:175:MET:CE       | 5:P:436:ALA:CB       | 2.70                     | 0.61              |
| 6:O8:180:GLY:C       | 6:O8:182:GLU:N       | 2.59                     | 0.61              |
| 8:L:976:LEU:HD22     | 9:K:1004:ARG:HD3     | 1.81                     | 0.61              |
| 9:K:1028:GLN:OE1     | 9:K:1037:ALA:CA      | 2.47                     | 0.61              |
| 9:K16:894:LYS:HZ1    | 9:K16:1057:GLU:HB2   | 1.65                     | 0.61              |
| 9:K16:1198:LEU:HD22  | 9:K16:1267:LEU:HD13  | 1.82                     | 0.61              |
| 10:C16:792:PHE:CD1   | 10:C16:850:ARG:NH1   | 2.68                     | 0.61              |
| 10:C16:1278:ASP:OD2  | 21:H:283:LYS:CG      | 2.48                     | 0.61              |
| 10:C16:1660:SER:C    | 10:C16:1662:ASP:H    | 2.08                     | 0.61              |
| 10:C24:667:ILE:HG12  | 10:C24:670:GLU:N     | 2.14                     | 0.61              |
| 10:C24:1211:VAL:HG13 | 10:C24:1232:ILE:HD13 | 1.82                     | 0.61              |
| 10:C24:1583:ILE:HD11 | 10:C24:1631:LYS:HB3  | 1.83                     | 0.61              |
| 14:W:711:ARG:CZ      | 10:C8:1606:GLY:O     | 2.42                     | 0.61              |
| 14:W:746:THR:HG23    | 15:J:675:ASN:ND2     | 2.15                     | 0.61              |
| 10:C8:453:LEU:CB     | 10:C8:486:LEU:HD21   | 2.29                     | 0.61              |
| 10:C8:556:VAL:HG12   | 10:C8:565:ARG:NH1    | 2.15                     | 0.61              |
| 10:C8:792:PHE:CD1    | 10:C8:850:ARG:NH1    | 2.68                     | 0.61              |
| 10:C8:1061:ASN:O     | 10:C8:1062:GLU:C     | 2.25                     | 0.61              |
| 10:C8:1211:VAL:HG13  | 10:C8:1232:ILE:HD13  | 1.82                     | 0.61              |
| 10:C8:1234:ASP:OD1   | 10:C8:1302:LYS:NZ    | 2.25                     | 0.61              |
| 11:A16:668:HIS:HE1   | 11:A16:672:GLU:OE1   | 1.82                     | 0.61              |
| 18:B:395:ARG:HB2     | 18:B:426:VAL:HG11    | 1.80                     | 0.61              |
| 18:B8:627:SER:O      | 18:B8:631:LEU:HG     | 2.00                     | 0.61              |
| 18:B8:1694:GLU:OE2   | 18:B8:1822:GLN:NE2   | 2.29                     | 0.61              |
| 21:H8:291:VAL:HG22   | 22:I8:273:LEU:HD21   | 1.81                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:J16:688:PRO:O    | 23:J16:692:VAL:HG23 | 2.00                     | 0.61              |
| 24:D:409:LEU:CG     | 24:D16:746:ALA:H    | 2.14                     | 0.61              |
| 24:D8:758:ALA:HB1   | 24:D8:759:TYR:CD2   | 2.36                     | 0.61              |
| 10:C32:105:TRP:O    | 10:C32:932:LYS:O    | 2.17                     | 0.61              |
| 10:C32:1278:ASP:O   | 10:C32:1734:ARG:NH1 | 2.32                     | 0.61              |
| 10:C32:1660:SER:C   | 10:C32:1662:ASP:H   | 2.08                     | 0.61              |
| 12:A48:437:LEU:CD1  | 12:A48:454:LYS:HZ3  | 2.12                     | 0.61              |
| 2:M:358:LEU:HB2     | 2:M:359:PRO:HD3     | 1.81                     | 0.61              |
| 5:P16:47:ASN:H      | 5:P16:471:SER:HG    | 1.48                     | 0.61              |
| 5:P16:394:ASN:O     | 5:P16:396:SER:N     | 2.29                     | 0.61              |
| 7:Q16:221:TRP:CE3   | 7:Q16:222:PHE:CE2   | 2.87                     | 0.61              |
| 9:K8:853:ALA:HB2    | 9:K8:856:ILE:HD12   | 1.80                     | 0.61              |
| 9:K8:994:TYR:CD2    | 9:K8:1023:LEU:CD1   | 2.83                     | 0.61              |
| 10:C16:1618:SER:C   | 10:C16:1620:ILE:H   | 2.06                     | 0.61              |
| 10:C24:16:LEU:CD2   | 10:C24:139:ARG:HH12 | 2.12                     | 0.61              |
| 11:A40:156:MET:HA   | 11:A40:555:HIS:NE2  | 2.15                     | 0.61              |
| 12:A:288:HIS:HB2    | 12:A:354:ARG:HH12   | 1.64                     | 0.61              |
| 13:V:811:MET:HE1    | 14:W:698:LEU:HB3    | 1.81                     | 0.61              |
| 10:C:33:ILE:CG2     | 10:C:158:LEU:HD22   | 2.30                     | 0.61              |
| 18:B:810:THR:OG1    | 18:B:879:SER:O      | 2.17                     | 0.61              |
| 18:B:1888:ILE:HD11  | 18:B:1943:HIS:CE1   | 2.35                     | 0.61              |
| 18:B8:1161:LEU:CD1  | 18:B8:1403:ILE:CD1  | 2.76                     | 0.61              |
| 21:H16:291:VAL:HG22 | 22:I16:273:LEU:HD21 | 1.81                     | 0.61              |
| 24:D24:758:ALA:HB1  | 24:D24:759:TYR:CD2  | 2.36                     | 0.61              |
| 10:C32:275:ALA:HB1  | 10:C32:326:LEU:HD12 | 1.82                     | 0.61              |
| 1:R:1033:LYS:NZ     | 24:D:1432:THR:CG2   | 2.60                     | 0.61              |
| 2:M:343:MET:C       | 2:M:345:ASP:N       | 2.56                     | 0.61              |
| 2:M8:358:LEU:HB2    | 2:M8:359:PRO:HD3    | 1.81                     | 0.61              |
| 2:M16:738:ILE:HD11  | 2:M16:779:SER:CB    | 2.30                     | 0.61              |
| 7:Q:136:ARG:NH1     | 7:Q:138:GLU:OE2     | 2.34                     | 0.61              |
| 5:P8:101:LEU:HD22   | 5:P8:133:TYR:CE2    | 2.36                     | 0.61              |
| 7:Q16:272:SER:C     | 7:Q16:274:ASN:N     | 2.58                     | 0.61              |
| 9:K:840:TRP:CE3     | 9:K:907:ILE:HD11    | 2.33                     | 0.61              |
| 9:K8:1139:ILE:O     | 9:K8:1140:GLN:C     | 2.39                     | 0.61              |
| 10:C16:768:ARG:CZ   | 10:C16:775:LYS:CG   | 2.69                     | 0.61              |
| 10:C16:1074:LEU:O   | 10:C16:1076:TYR:N   | 2.33                     | 0.61              |
| 10:C24:390:HIS:CE1  | 10:C24:449:GLU:OE2  | 2.53                     | 0.61              |
| 10:C24:407:LYS:HG3  | 10:C24:465:PHE:HE1  | 1.64                     | 0.61              |
| 10:C24:1010:ALA:H   | 10:C24:1192:ARG:NH2 | 1.63                     | 0.61              |
| 11:A32:668:HIS:HE1  | 11:A32:672:GLU:OE1  | 1.82                     | 0.61              |
| 18:B8:750:GLU:HG3   | 18:B8:760:ARG:NH2   | 2.15                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B8:1205:ILE:HD11 | 18:B8:1271:PHE:CE2  | 2.33                     | 0.61              |
| 21:H8:255:LEU:HD12  | 23:J8:655:GLU:CD    | 2.22                     | 0.61              |
| 22:I8:368:VAL:HG22  | 23:J8:591:LYS:CE    | 2.30                     | 0.61              |
| 23:J8:688:PRO:O     | 23:J8:692:VAL:HG23  | 2.00                     | 0.61              |
| 21:H24:361:ARG:NH2  | 22:I24:354:ASP:OD1  | 2.32                     | 0.61              |
| 21:H16:312:GLN:NE2  | 22:I16:290:ASP:CG   | 2.57                     | 0.61              |
| 10:C32:847:ARG:NH2  | 10:C32:910:SER:CB   | 2.59                     | 0.61              |
| 1:R:1266:THR:HA     | 5:P:684:ARG:NH2     | 2.13                     | 0.61              |
| 1:R8:1190:VAL:HG22  | 24:D40:1456:GLU:C   | 2.25                     | 0.61              |
| 1:R16:634:ARG:CG    | 4:T16:160:HIS:CE1   | 2.84                     | 0.61              |
| 1:R16:1165:MET:HE3  | 1:R16:1220:GLN:HG3  | 1.80                     | 0.61              |
| 8:L8:598:LEU:CD2    | 8:L8:627:ARG:CZ     | 2.78                     | 0.61              |
| 9:K:787:PRO:HG2     | 9:K:790:THR:OG1     | 1.99                     | 0.61              |
| 9:K:1139:ILE:O      | 9:K:1140:GLN:C      | 2.39                     | 0.61              |
| 10:C16:26:ARG:NH2   | 10:C16:148:GLU:OE2  | 2.33                     | 0.61              |
| 10:C16:296:PHE:CE1  | 10:C16:300:VAL:HG21 | 2.36                     | 0.61              |
| 11:A24:707:LEU:HD21 | 11:A24:767:ARG:HH22 | 1.59                     | 0.61              |
| 10:C24:792:PHE:CD1  | 10:C24:850:ARG:NH1  | 2.68                     | 0.61              |
| 10:C24:1074:LEU:O   | 10:C24:1076:TYR:N   | 2.33                     | 0.61              |
| 11:A40:302:GLN:HE21 | 11:A40:324:ARG:NH1  | 1.97                     | 0.61              |
| 11:A40:749:GLN:HE21 | 24:D24:1398:ARG:NE  | 1.98                     | 0.61              |
| 12:A:388:VAL:HG23   | 12:A:459:ARG:NH1    | 2.12                     | 0.61              |
| 13:V:790:GLN:HE22   | 14:W:674:GLN:CD     | 2.06                     | 0.61              |
| 10:C8:668:ALA:HA    | 10:C8:700:MET:HE3   | 1.76                     | 0.61              |
| 10:C8:959:GLU:HG2   | 10:C8:1139:ARG:HE   | 1.66                     | 0.61              |
| 10:C8:1278:ASP:O    | 10:C8:1734:ARG:NH1  | 2.32                     | 0.61              |
| 18:B:618:VAL:CG1    | 18:B:621:VAL:CG2    | 2.75                     | 0.61              |
| 18:B:1541:LEU:HD22  | 18:B:1576:MET:HE3   | 1.82                     | 0.61              |
| 18:B8:1528:PRO:HA   | 18:B8:1531:TRP:CE2  | 2.34                     | 0.61              |
| 20:E:473:LEU:HD11   | 20:E:514:PHE:HB3    | 1.82                     | 0.61              |
| 20:E8:434:TRP:CD1   | 24:D40:72:GLU:CG    | 2.83                     | 0.61              |
| 21:H:361:ARG:NH2    | 22:I:354:ASP:OD1    | 2.32                     | 0.61              |
| 21:H24:312:GLN:CG   | 21:H24:316:ILE:CD1  | 2.39                     | 0.61              |
| 21:H16:363:MET:SD   | 22:I16:332:MET:CE   | 2.80                     | 0.61              |
| 10:C32:26:ARG:NH2   | 10:C32:148:GLU:OE2  | 2.33                     | 0.61              |
| 10:C32:33:ILE:CG2   | 10:C32:158:LEU:HD22 | 2.30                     | 0.61              |
| 10:C32:565:ARG:CZ   | 10:C32:602:VAL:CG1  | 2.79                     | 0.61              |
| 12:A48:437:LEU:HD11 | 12:A48:454:LYS:HE2  | 1.81                     | 0.61              |
| 1:R:1369:LEU:HD13   | 6:O:211:ASN:CG      | 2.23                     | 0.61              |
| 1:R:1449:TRP:CH2    | 2:M:161:ASP:C       | 2.78                     | 0.61              |
| 5:P:30:TYR:HE2      | 5:P:32:LEU:HB2      | 1.64                     | 0.61              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 7:Q:219:GLY:HA2      | 7:Q:221:TRP:CD1      | 2.36                     | 0.61              |
| 5:P8:206:SER:OG      | 5:P8:207:HIS:CE1     | 2.54                     | 0.61              |
| 5:P16:97:SER:HB3     | 5:P16:98:PRO:HD3     | 1.83                     | 0.61              |
| 7:Q16:254:ALA:CB     | 7:Q16:302:ILE:HD13   | 2.30                     | 0.61              |
| 9:K:577:GLN:HG2      | 9:K:625:ARG:NH1      | 2.15                     | 0.61              |
| 9:K8:1046:LEU:O      | 9:K8:1048:GLN:N      | 2.33                     | 0.61              |
| 10:C16:798:VAL:CG1   | 10:C16:802:TRP:CZ2   | 2.83                     | 0.61              |
| 10:C16:1333:HIS:CE1  | 10:C16:1337:LEU:HD22 | 2.35                     | 0.61              |
| 10:C24:626:GLN:O     | 10:C24:627:VAL:C     | 2.38                     | 0.61              |
| 10:C24:1002:LEU:HD12 | 10:C24:1019:ARG:HH12 | 1.61                     | 0.61              |
| 10:C24:1015:SER:OG   | 10:C24:1019:ARG:NH1  | 2.33                     | 0.61              |
| 10:C24:1333:HIS:CE1  | 10:C24:1337:LEU:HD22 | 2.34                     | 0.61              |
| 12:A:634:ILE:CD1     | 12:A:678:LYS:HZ2     | 2.14                     | 0.61              |
| 14:W:646:ALA:HB3     | 14:W:647:PRO:HD3     | 1.82                     | 0.61              |
| 14:W:701:LEU:HD21    | 15:J:624:ALA:HB1     | 1.80                     | 0.61              |
| 10:C:26:ARG:NH2      | 10:C:148:GLU:OE2     | 2.33                     | 0.61              |
| 10:C:573:GLU:N       | 10:C:574:PRO:CD      | 2.64                     | 0.61              |
| 10:C:798:VAL:CG1     | 10:C:802:TRP:CZ2     | 2.84                     | 0.61              |
| 10:C8:275:ALA:HB1    | 10:C8:326:LEU:HD12   | 1.83                     | 0.61              |
| 10:C8:296:PHE:CE1    | 10:C8:300:VAL:HG21   | 2.36                     | 0.61              |
| 11:A16:676:TYR:CD2   | 24:D16:1396:PRO:HD2  | 2.33                     | 0.61              |
| 11:A32:302:GLN:HE21  | 11:A32:324:ARG:NH1   | 1.97                     | 0.61              |
| 18:B:750:GLU:HG3     | 18:B:760:ARG:NE      | 2.14                     | 0.61              |
| 18:B8:682:TYR:C      | 18:B8:684:ILE:H      | 2.08                     | 0.61              |
| 20:E:352:PHE:HE1     | 20:E:451:ILE:CD1     | 1.94                     | 0.61              |
| 20:E:414:MET:CE      | 20:E:455:TYR:CE2     | 2.84                     | 0.61              |
| 20:E8:437:SER:O      | 20:E8:439:MET:N      | 2.34                     | 0.61              |
| 21:H24:237:PHE:HB2   | 21:H24:238:PRO:HD3   | 1.83                     | 0.61              |
| 24:D:758:ALA:HB1     | 24:D:759:TYR:CD2     | 2.36                     | 0.61              |
| 2:M:844:VAL:CG2      | 4:T:660:LEU:HD11     | 2.28                     | 0.61              |
| 1:R8:1190:VAL:HG21   | 24:D40:1457:SER:HA   | 1.83                     | 0.61              |
| 5:P:206:SER:OG       | 5:P:207:HIS:CE1      | 2.54                     | 0.61              |
| 6:O:90:GLU:CD        | 6:O:98:LYS:NZ        | 2.58                     | 0.61              |
| 6:O:125:VAL:HG23     | 6:O:175:TRP:HZ2      | 1.65                     | 0.61              |
| 7:Q:10:VAL:HG21      | 7:Q:327:LEU:HD21     | 1.82                     | 0.61              |
| 6:O16:125:VAL:HG23   | 6:O16:175:TRP:HZ2    | 1.65                     | 0.61              |
| 7:Q16:10:VAL:HG21    | 7:Q16:327:LEU:HD21   | 1.82                     | 0.61              |
| 7:Q16:297:VAL:CG2    | 7:Q16:318:GLU:OE1    | 2.48                     | 0.61              |
| 10:C16:573:GLU:N     | 10:C16:574:PRO:CD    | 2.64                     | 0.61              |
| 10:C16:1583:ILE:HD11 | 10:C16:1631:LYS:HB3  | 1.83                     | 0.61              |
| 10:C16:1821:VAL:HG11 | 11:A24:144:LYS:HE3   | 1.82                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A24:493:TYR:OH   | 17:F:57:PRO:O       | 2.17                     | 0.61              |
| 10:C24:698:PHE:CZ   | 10:C24:749:LEU:HD11 | 2.36                     | 0.61              |
| 11:A40:388:VAL:HG23 | 11:A40:459:ARG:NH1  | 2.12                     | 0.61              |
| 12:A:144:LYS:HE3    | 10:C:1821:VAL:HG11  | 1.81                     | 0.61              |
| 10:C:1074:LEU:O     | 10:C:1076:TYR:N     | 2.33                     | 0.61              |
| 10:C8:1805:ASP:OD1  | 10:C8:1830:LYS:NZ   | 2.27                     | 0.61              |
| 11:A16:148:LEU:HD13 | 18:B:1956:ILE:HD13  | 1.83                     | 0.61              |
| 11:A16:388:VAL:HG23 | 11:A16:459:ARG:NH1  | 2.12                     | 0.61              |
| 11:A32:148:LEU:HD13 | 18:B8:1956:ILE:HD13 | 1.83                     | 0.61              |
| 18:B:112:GLU:OE2    | 18:B:130:MET:CE     | 2.44                     | 0.61              |
| 18:B:457:SER:HA     | 18:B:548:ARG:HH12   | 1.59                     | 0.61              |
| 18:B:712:PRO:HG3    | 18:B:759:MET:CE     | 2.23                     | 0.61              |
| 18:B:1694:GLU:OE2   | 18:B:1822:GLN:NE2   | 2.29                     | 0.61              |
| 19:4:55:GLN:C       | 19:4:57:ASN:H       | 2.09                     | 0.61              |
| 10:C32:389:LEU:HD23 | 10:C32:447:PHE:CE1  | 2.35                     | 0.61              |
| 2:M:367:SER:HB2     | 2:M:486:MET:CE      | 2.31                     | 0.61              |
| 2:M:672:TYR:CD2     | 2:M:680:LYS:HD3     | 2.35                     | 0.61              |
| 4:T8:156:SER:O      | 4:T8:160:HIS:CE1    | 2.53                     | 0.61              |
| 5:P:30:TYR:CE2      | 5:P:32:LEU:HB2      | 2.36                     | 0.61              |
| 5:P:507:GLN:NE2     | 7:Q:136:ARG:NH2     | 2.49                     | 0.61              |
| 7:Q8:219:GLY:HA2    | 7:Q8:221:TRP:CD1    | 2.36                     | 0.61              |
| 5:P16:206:SER:OG    | 5:P16:207:HIS:CE1   | 2.54                     | 0.61              |
| 7:Q16:219:GLY:HA2   | 7:Q16:221:TRP:CD1   | 2.36                     | 0.61              |
| 7:Q16:236:HIS:CE1   | 7:Q16:238:SER:OG    | 2.53                     | 0.61              |
| 8:L16:947:ASN:HB3   | 8:L16:1026:ARG:CZ   | 2.31                     | 0.61              |
| 9:K8:722:GLN:O      | 9:K8:723:ALA:C      | 2.38                     | 0.61              |
| 9:K8:1048:GLN:NE2   | 9:K8:1128:ARG:CG    | 2.62                     | 0.61              |
| 10:C16:698:PHE:CZ   | 10:C16:749:LEU:HD11 | 2.36                     | 0.61              |
| 10:C16:1547:LYS:NZ  | 24:D8:1405:GLY:CA   | 2.61                     | 0.61              |
| 11:A24:668:HIS:HE1  | 11:A24:672:GLU:OE1  | 1.82                     | 0.61              |
| 10:C24:296:PHE:CE1  | 10:C24:300:VAL:HG21 | 2.35                     | 0.61              |
| 10:C24:1318:ARG:NH2 | 10:C24:1396:SER:CB  | 2.62                     | 0.61              |
| 10:C24:1660:SER:C   | 10:C24:1662:ASP:H   | 2.08                     | 0.61              |
| 10:C24:1693:LYS:NZ  | 10:C24:1749:ASP:OD1 | 2.33                     | 0.61              |
| 11:A40:683:GLN:OE1  | 11:A40:692:ALA:HA   | 2.00                     | 0.61              |
| 13:V:861:PHE:CZ     | 14:W:742:VAL:HG22   | 2.32                     | 0.61              |
| 14:W:591:LEU:CD2    | 15:J:566:ASN:OD1    | 2.46                     | 0.61              |
| 10:C:296:PHE:CE1    | 10:C:300:VAL:HG21   | 2.36                     | 0.61              |
| 11:A16:683:GLN:OE1  | 11:A16:692:ALA:HA   | 2.00                     | 0.61              |
| 11:A32:112:ALA:CB   | 18:B8:1416:LYS:HZ3  | 2.14                     | 0.61              |
| 18:B:1548:LEU:HD11  | 18:B:1564:PHE:CE2   | 2.35                     | 0.61              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B8:410:GLN:CD     | 18:B8:538:ARG:HH22  | 2.09                     | 0.61              |
| 18:B8:864:LEU:HB3    | 18:B8:910:TYR:CE2   | 2.36                     | 0.61              |
| 18:B8:1541:LEU:HD22  | 18:B8:1576:MET:HE3  | 1.82                     | 0.61              |
| 19:4:65:LYS:O        | 19:4:66:ALA:O       | 2.19                     | 0.61              |
| 19:4:306:ASP:OD1     | 19:4:307:PRO:CD     | 2.49                     | 0.61              |
| 20:E:429:PRO:HB2     | 24:D:69:VAL:HG22    | 1.80                     | 0.61              |
| 19:48:352:CYS:SG     | 19:48:371:TYR:HB2   | 2.40                     | 0.61              |
| 22:I:268:ARG:CG      | 22:I:272:TYR:CE2    | 2.84                     | 0.61              |
| 21:H24:363:MET:SD    | 22:I24:332:MET:CE   | 2.81                     | 0.61              |
| 23:J24:688:PRO:O     | 23:J24:692:VAL:HG23 | 2.00                     | 0.61              |
| 24:D16:758:ALA:HB1   | 24:D16:759:TYR:CD2  | 2.36                     | 0.61              |
| 10:C32:1358:ASP:O    | 10:C32:1361:LYS:N   | 2.31                     | 0.61              |
| 1:R:1388:GLY:O       | 3:N:56:ARG:HB3      | 2.01                     | 0.61              |
| 2:M:627:TYR:CZ       | 3:N:162:THR:HB      | 2.35                     | 0.61              |
| 1:R8:1449:TRP:CH2    | 2:M8:160:LEU:CD1    | 2.82                     | 0.61              |
| 2:M8:755:THR:C       | 2:M8:757:VAL:N      | 2.57                     | 0.61              |
| 2:M16:342:VAL:CG1    | 2:M16:343:MET:N     | 2.59                     | 0.61              |
| 2:M16:627:TYR:N      | 2:M16:627:TYR:CD2   | 2.52                     | 0.61              |
| 6:O:61:LYS:NZ        | 6:O:112:ASP:CG      | 2.48                     | 0.61              |
| 6:O:180:GLY:C        | 6:O:182:GLU:N       | 2.59                     | 0.61              |
| 7:Q8:241:HIS:CD2     | 7:Q8:258:ARG:CZ     | 2.81                     | 0.61              |
| 8:L16:1069:LEU:HD21  | 9:K16:1086:VAL:CG2  | 2.31                     | 0.61              |
| 9:K:842:ILE:HG23     | 9:K:871:LEU:HD21    | 1.82                     | 0.61              |
| 10:C16:1111:SER:C    | 10:C16:1113:LYS:N   | 2.58                     | 0.61              |
| 10:C24:386:ASN:OD1   | 10:C24:449:GLU:OE1  | 2.18                     | 0.61              |
| 10:C24:1548:ILE:HG12 | 24:D24:1407:PHE:HE2 | 1.62                     | 0.61              |
| 12:A:437:LEU:HD11    | 12:A:454:LYS:HE2    | 1.81                     | 0.61              |
| 10:C:62:ILE:CD1      | 10:C:72:LEU:CD1     | 2.73                     | 0.61              |
| 10:C:1061:ASN:O      | 10:C:1062:GLU:C     | 2.25                     | 0.61              |
| 10:C8:1121:ILE:CG2   | 10:C8:1133:ILE:CD1  | 2.77                     | 0.61              |
| 10:C8:1234:ASP:CG    | 10:C8:1302:LYS:HZ2  | 2.09                     | 0.61              |
| 10:C8:1290:HIS:HD2   | 10:C8:1334:MET:HE2  | 1.66                     | 0.61              |
| 18:B:503:SER:N       | 18:B:504:PRO:CD     | 2.63                     | 0.61              |
| 18:B:1548:LEU:HD11   | 18:B:1564:PHE:HE2   | 1.65                     | 0.61              |
| 19:48:180:ALA:CB     | 19:48:202:ILE:HD11  | 2.14                     | 0.61              |
| 21:H8:243:LEU:CD1    | 23:J8:603:LEU:HG    | 2.31                     | 0.61              |
| 22:I8:203:GLN:N      | 22:I8:204:PRO:CD    | 2.64                     | 0.61              |
| 22:I16:203:GLN:N     | 22:I16:204:PRO:CD   | 2.64                     | 0.61              |
| 24:D32:749:ARG:NH2   | 24:D40:397:ALA:N    | 2.31                     | 0.61              |
| 10:C32:643:LEU:CD1   | 10:C32:679:ARG:HH12 | 2.03                     | 0.61              |
| 10:C32:1015:SER:OG   | 10:C32:1019:ARG:NH1 | 2.33                     | 0.61              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 12:A48:668:HIS:HE1  | 12:A48:672:GLU:OE1   | 1.82                     | 0.61              |
| 1:R:1225:PHE:CD2    | 1:R:1241:TYR:CE2     | 2.88                     | 0.60              |
| 1:R16:1388:GLY:O    | 3:N16:56:ARG:HB3     | 2.01                     | 0.60              |
| 5:P8:30:TYR:CE2     | 5:P8:32:LEU:HB2      | 2.36                     | 0.60              |
| 5:P16:105:ARG:HG2   | 5:P16:126:TRP:CZ2    | 2.36                     | 0.60              |
| 6:O16:133:LEU:HD21  | 6:O16:153:PHE:CE2    | 2.36                     | 0.60              |
| 8:L:1041:SER:HB2    | 8:L:1054:HIS:CE1     | 2.34                     | 0.60              |
| 9:K:994:TYR:CD2     | 9:K:1023:LEU:CD1     | 2.83                     | 0.60              |
| 10:C16:389:LEU:HD23 | 10:C16:447:PHE:CE1   | 2.35                     | 0.60              |
| 10:C16:717:GLU:O    | 10:C16:719:PRO:N     | 2.34                     | 0.60              |
| 11:A40:803:PRO:CG   | 24:D24:1401:LEU:HD12 | 2.30                     | 0.60              |
| 12:A:683:GLN:OE1    | 12:A:692:ALA:HA      | 2.00                     | 0.60              |
| 10:C:150:ASP:OD1    | 24:D:1404:GLY:HA3    | 1.99                     | 0.60              |
| 10:C:717:GLU:O      | 10:C:719:PRO:N       | 2.34                     | 0.60              |
| 10:C8:573:GLU:N     | 10:C8:574:PRO:CD     | 2.64                     | 0.60              |
| 10:C8:1015:SER:OG   | 10:C8:1019:ARG:NH1   | 2.33                     | 0.60              |
| 11:A32:703:ALA:CA   | 24:D32:1398:ARG:HD3  | 2.20                     | 0.60              |
| 18:B:1856:PHE:CD1   | 18:B:1857:PRO:HD2    | 2.36                     | 0.60              |
| 18:B8:1152:ASP:CG   | 18:B8:1378:LYS:NZ    | 2.57                     | 0.60              |
| 18:B8:1888:ILE:HD11 | 18:B8:1943:HIS:CE1   | 2.35                     | 0.60              |
| 19:4:350:THR:O      | 19:4:374:GLY:HA2     | 2.00                     | 0.60              |
| 20:E:91:ASP:OD1     | 20:E:92:PRO:HD2      | 2.01                     | 0.60              |
| 19:48:65:LYS:O      | 19:48:66:ALA:O       | 2.19                     | 0.60              |
| 20:E8:414:MET:CE    | 20:E8:455:TYR:CE2    | 2.84                     | 0.60              |
| 21:H8:139:ASP:OD1   | 21:H8:140:PRO:CD     | 2.34                     | 0.60              |
| 21:H8:366:MET:HE1   | 22:I8:332:MET:HE2    | 1.83                     | 0.60              |
| 21:H24:139:ASP:OD1  | 21:H24:140:PRO:CD    | 2.34                     | 0.60              |
| 22:I24:368:VAL:HG22 | 23:J24:591:LYS:CE    | 2.31                     | 0.60              |
| 24:D:406:ASN:HD21   | 24:D16:9:MET:HB2     | 1.65                     | 0.60              |
| 10:C32:717:GLU:O    | 10:C32:719:PRO:N     | 2.34                     | 0.60              |
| 10:C32:1061:ASN:O   | 10:C32:1063:PRO:N    | 2.34                     | 0.60              |
| 12:A48:560:MET:CE   | 12:A48:615:GLN:CD    | 2.73                     | 0.60              |
| 1:R8:1388:GLY:O     | 3:N8:56:ARG:HB3      | 2.01                     | 0.60              |
| 2:M8:401:ARG:NH2    | 8:L8:381:GLU:HB3     | 2.15                     | 0.60              |
| 1:R16:1225:PHE:CD2  | 1:R16:1241:TYR:CE2   | 2.89                     | 0.60              |
| 2:M16:173:SER:OG    | 3:N16:234:GLN:NE2    | 2.31                     | 0.60              |
| 2:M16:377:ARG:NH1   | 2:M16:477:ASP:CG     | 2.59                     | 0.60              |
| 7:Q8:236:HIS:CE1    | 7:Q8:238:SER:OG      | 2.53                     | 0.60              |
| 8:L16:1068:PHE:CD1  | 8:L16:1068:PHE:C     | 2.79                     | 0.60              |
| 11:A24:212:LYS:NZ   | 11:A24:585:MET:HE3   | 2.16                     | 0.60              |
| 10:C24:573:GLU:N    | 10:C24:574:PRO:CD    | 2.64                     | 0.60              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:1283:LEU:O    | 10:C24:1287:MET:N    | 2.33                     | 0.60              |
| 10:C24:1290:HIS:CB   | 10:C24:1334:MET:CE   | 2.72                     | 0.60              |
| 10:C24:1465:LEU:O    | 10:C24:1469:HIS:ND1  | 2.34                     | 0.60              |
| 11:A40:156:MET:CG    | 11:A40:555:HIS:CE1   | 2.67                     | 0.60              |
| 11:A40:468:VAL:CG2   | 24:D32:1103:LEU:HD11 | 2.17                     | 0.60              |
| 14:W:518:GLU:N       | 14:W:605:ASN:HD21    | 1.98                     | 0.60              |
| 10:C:1318:ARG:NH2    | 10:C:1396:SER:CB     | 2.63                     | 0.60              |
| 18:B:410:GLN:CD      | 18:B:538:ARG:HH22    | 2.09                     | 0.60              |
| 18:B8:1447:SER:O     | 18:B8:1447:SER:OG    | 2.20                     | 0.60              |
| 21:H:244:ARG:NH2     | 22:I:177:VAL:CG1     | 2.65                     | 0.60              |
| 22:I24:97:THR:HG22   | 22:I24:107:THR:HG21  | 1.81                     | 0.60              |
| 10:C32:663:ILE:HG22  | 10:C32:667:ILE:CG2   | 2.31                     | 0.60              |
| 10:C32:966:CYS:HA    | 10:C32:1025:LEU:HD12 | 1.83                     | 0.60              |
| 2:M:627:TYR:CG       | 3:N:167:LEU:HA       | 2.36                     | 0.60              |
| 2:M:776:LEU:HD23     | 2:M:795:TYR:CD2      | 2.35                     | 0.60              |
| 1:R8:1466:LYS:HD2    | 6:O8:160:LEU:CD1     | 2.31                     | 0.60              |
| 2:M8:627:TYR:CZ      | 3:N8:162:THR:HB      | 2.35                     | 0.60              |
| 2:M16:593:HIS:CD2    | 3:N16:224:LEU:CD2    | 2.84                     | 0.60              |
| 2:M16:666:GLU:HA     | 2:M16:684:GLN:OE1    | 2.01                     | 0.60              |
| 5:P:16:PHE:CZ        | 5:P:461:HIS:NE2      | 2.70                     | 0.60              |
| 5:P8:97:SER:HB3      | 5:P8:98:PRO:HD3      | 1.82                     | 0.60              |
| 5:P16:187:TRP:CZ3    | 5:P16:191:ARG:CD     | 2.84                     | 0.60              |
| 9:K:635:ALA:O        | 9:K:638:TRP:NE1      | 2.32                     | 0.60              |
| 10:C16:667:ILE:HG12  | 10:C16:670:GLU:N     | 2.14                     | 0.60              |
| 10:C16:1015:SER:OG   | 10:C16:1019:ARG:NH1  | 2.33                     | 0.60              |
| 10:C24:1023:LEU:HA   | 10:C24:1210:ILE:HD11 | 1.84                     | 0.60              |
| 10:C24:1163:LEU:HD23 | 10:C24:1166:SER:HG   | 1.61                     | 0.60              |
| 10:C24:1660:SER:C    | 10:C24:1662:ASP:N    | 2.59                     | 0.60              |
| 10:C8:798:VAL:CG1    | 10:C8:802:TRP:CZ2    | 2.84                     | 0.60              |
| 11:A32:683:GLN:OE1   | 11:A32:692:ALA:HA    | 2.00                     | 0.60              |
| 18:B:627:SER:O       | 18:B:631:LEU:HG      | 2.00                     | 0.60              |
| 18:B:1505:MET:HE3    | 18:B:1518:VAL:HG21   | 1.82                     | 0.60              |
| 18:B8:1424:LEU:HD22  | 18:B8:1490:ILE:HD12  | 1.82                     | 0.60              |
| 20:E:52:VAL:CG1      | 20:E:121:VAL:HG21    | 2.31                     | 0.60              |
| 19:48:55:GLN:C       | 19:48:57:ASN:N       | 2.60                     | 0.60              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:CE2    | 2.76                     | 0.60              |
| 21:H:243:LEU:CD1     | 23:J32:603:LEU:HG    | 2.31                     | 0.60              |
| 24:D40:843:GLN:NE2   | 24:D40:971:HIS:ND1   | 2.49                     | 0.60              |
| 12:A48:683:GLN:OE1   | 12:A48:692:ALA:HA    | 2.00                     | 0.60              |
| 1:R:909:GLN:HE21     | 24:D:1361:ALA:HB2    | 1.66                     | 0.60              |
| 1:R:1428:VAL:CG2     | 6:O:165:LYS:HZ1      | 2.11                     | 0.60              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 3:N:222:LEU:HD11    | 3:N:270:THR:HA       | 1.81                     | 0.60              |
| 2:M8:349:ASP:C      | 2:M8:351:ALA:H       | 2.09                     | 0.60              |
| 2:M8:428:SER:CB     | 8:L8:355:SER:HG      | 1.77                     | 0.60              |
| 1:R16:1349:ARG:HG3  | 1:R16:1390:GLU:OE2   | 2.01                     | 0.60              |
| 2:M16:354:ASP:C     | 2:M16:356:GLU:H      | 2.08                     | 0.60              |
| 2:M16:367:SER:HB2   | 2:M16:486:MET:CE     | 2.31                     | 0.60              |
| 6:O:90:GLU:CD       | 6:O:98:LYS:HZ2       | 2.10                     | 0.60              |
| 7:Q:254:ALA:CB      | 7:Q:302:ILE:HD13     | 2.30                     | 0.60              |
| 5:P8:187:TRP:CZ3    | 5:P8:191:ARG:CD      | 2.84                     | 0.60              |
| 5:P16:56:ASN:CB     | 5:P16:59:LEU:HD12    | 2.27                     | 0.60              |
| 7:Q16:136:ARG:NH1   | 7:Q16:138:GLU:OE2    | 2.33                     | 0.60              |
| 8:L16:601:HIS:CE1   | 8:L16:631:LEU:HD22   | 2.36                     | 0.60              |
| 10:C16:123:TRP:CH2  | 10:C16:127:ARG:HD2   | 2.37                     | 0.60              |
| 10:C16:1023:LEU:HA  | 10:C16:1210:ILE:HD11 | 1.84                     | 0.60              |
| 14:W:586:ILE:CG1    | 15:J:572:ASP:CB      | 2.79                     | 0.60              |
| 10:C:698:PHE:CZ     | 10:C:749:LEU:HD11    | 2.36                     | 0.60              |
| 11:A16:120:ALA:HB1  | 18:B:1520:LEU:CD1    | 2.31                     | 0.60              |
| 11:A16:302:GLN:HE21 | 11:A16:324:ARG:NH1   | 1.97                     | 0.60              |
| 18:B8:1081:LEU:CD1  | 18:B8:1337:SER:OG    | 2.49                     | 0.60              |
| 18:B8:1129:LYS:O    | 18:B8:1131:THR:N     | 2.34                     | 0.60              |
| 18:B8:1548:LEU:HD11 | 18:B8:1564:PHE:HE2   | 1.65                     | 0.60              |
| 20:E8:52:VAL:CG1    | 20:E8:121:VAL:HG21   | 2.31                     | 0.60              |
| 20:E8:91:ASP:OD1    | 20:E8:92:PRO:HD2     | 2.01                     | 0.60              |
| 22:I:368:VAL:HG22   | 23:J32:591:LYS:CE    | 2.31                     | 0.60              |
| 22:I8:207:PRO:C     | 22:I8:209:TRP:N      | 2.60                     | 0.60              |
| 21:H24:243:LEU:CD1  | 23:J24:603:LEU:HG    | 2.31                     | 0.60              |
| 21:H16:255:LEU:HD12 | 23:J16:655:GLU:CD    | 2.23                     | 0.60              |
| 10:C32:123:TRP:CH2  | 10:C32:127:ARG:HD2   | 2.37                     | 0.60              |
| 2:M8:278:VAL:HG11   | 2:M8:326:GLN:HG3     | 1.84                     | 0.60              |
| 2:M8:367:SER:HB2    | 2:M8:486:MET:CE      | 2.31                     | 0.60              |
| 1:R16:634:ARG:HG3   | 4:T16:160:HIS:CE1    | 2.37                     | 0.60              |
| 3:N16:97:HIS:CD2    | 3:N16:99:PHE:CE1     | 2.90                     | 0.60              |
| 5:P:451:LYS:CD      | 6:O:312:ASN:O        | 2.50                     | 0.60              |
| 5:P8:47:ASN:OD1     | 5:P8:471:SER:CB      | 2.50                     | 0.60              |
| 6:O8:125:VAL:HG23   | 6:O8:175:TRP:HZ2     | 1.65                     | 0.60              |
| 5:P16:451:LYS:CD    | 6:O16:312:ASN:O      | 2.50                     | 0.60              |
| 7:Q16:200:PHE:CZ    | 7:Q16:228:ALA:HA     | 2.37                     | 0.60              |
| 9:K:649:MET:CB      | 9:K:704:ARG:HH21     | 1.93                     | 0.60              |
| 9:K:916:LYS:O       | 9:K:919:MET:CG       | 2.37                     | 0.60              |
| 10:C16:847:ARG:O    | 10:C16:906:ARG:NH1   | 2.34                     | 0.60              |
| 11:A40:212:LYS:NZ   | 11:A40:585:MET:HE3   | 2.17                     | 0.60              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A40:668:HIS:HE1  | 11:A40:672:GLU:OE1   | 1.82                     | 0.60              |
| 12:A:115:SER:CB     | 10:C:1265:ARG:HH22   | 2.15                     | 0.60              |
| 10:C:123:TRP:CH2    | 10:C:127:ARG:HD2     | 2.36                     | 0.60              |
| 10:C:1061:ASN:O     | 10:C:1063:PRO:N      | 2.34                     | 0.60              |
| 10:C:1660:SER:C     | 10:C:1662:ASP:N      | 2.59                     | 0.60              |
| 10:C8:1318:ARG:NH2  | 10:C8:1396:SER:CB    | 2.63                     | 0.60              |
| 11:A16:501:PRO:HB2  | 11:A16:524:GLU:OE1   | 1.99                     | 0.60              |
| 11:A16:706:SER:OG   | 24:D16:1398:ARG:HB3  | 2.00                     | 0.60              |
| 18:B:789:LEU:CD2    | 18:B:793:LEU:HD12    | 2.19                     | 0.60              |
| 18:B:864:LEU:HB3    | 18:B:910:TYR:CE2     | 2.36                     | 0.60              |
| 18:B:1081:LEU:CD1   | 18:B:1337:SER:OG     | 2.49                     | 0.60              |
| 18:B:1447:SER:O     | 18:B:1447:SER:OG     | 2.20                     | 0.60              |
| 20:E:447:ILE:CG2    | 20:E:451:ILE:HG21    | 2.32                     | 0.60              |
| 19:48:29:ARG:O      | 19:48:33:THR:OG1     | 2.17                     | 0.60              |
| 21:H8:237:PHE:HB2   | 21:H8:238:PRO:HD3    | 1.83                     | 0.60              |
| 10:C32:626:GLN:O    | 10:C32:627:VAL:C     | 2.38                     | 0.60              |
| 10:C32:698:PHE:CZ   | 10:C32:749:LEU:HD11  | 2.36                     | 0.60              |
| 1:R:634:ARG:HG3     | 4:T:160:HIS:CE1      | 2.37                     | 0.60              |
| 2:M:385:LEU:CD1     | 2:M:396:PHE:CD2      | 2.83                     | 0.60              |
| 2:M:417:ARG:HA      | 8:L:346:TRP:CZ2      | 2.36                     | 0.60              |
| 2:M:614:TYR:CE2     | 2:M:618:HIS:HE1      | 2.20                     | 0.60              |
| 3:N:97:HIS:CD2      | 3:N:99:PHE:CE1       | 2.90                     | 0.60              |
| 1:R8:634:ARG:CG     | 4:T8:160:HIS:CE1     | 2.84                     | 0.60              |
| 1:R16:1115:TYR:CB   | 1:R16:1131:MET:HE3   | 2.32                     | 0.60              |
| 5:P:187:TRP:CZ3     | 5:P:191:ARG:CD       | 2.84                     | 0.60              |
| 5:P:303:LYS:HB3     | 5:P:304:PRO:HD3      | 1.84                     | 0.60              |
| 7:Q8:10:VAL:HG21    | 7:Q8:327:LEU:HD21    | 1.82                     | 0.60              |
| 7:Q8:200:PHE:CZ     | 7:Q8:228:ALA:HA      | 2.37                     | 0.60              |
| 9:K8:955:TYR:OH     | 9:K8:984:GLY:C       | 2.45                     | 0.60              |
| 10:C16:619:LEU:CB   | 10:C16:620:PRO:CD    | 2.79                     | 0.60              |
| 10:C16:1453:ARG:NH1 | 24:D8:1150:GLY:HA3   | 2.17                     | 0.60              |
| 10:C16:1660:SER:C   | 10:C16:1662:ASP:N    | 2.58                     | 0.60              |
| 10:C24:1530:PHE:O   | 10:C24:1533:THR:OG1  | 2.20                     | 0.60              |
| 10:C24:1615:PHE:HB3 | 10:C24:1674:LEU:HD23 | 1.84                     | 0.60              |
| 12:A:212:LYS:NZ     | 12:A:585:MET:HE3     | 2.16                     | 0.60              |
| 13:V:880:ARG:O      | 13:V:881:GLY:C       | 2.40                     | 0.60              |
| 10:C:768:ARG:CZ     | 10:C:775:LYS:CG      | 2.69                     | 0.60              |
| 10:C:898:GLN:NE2    | 10:C:1138:GLU:CD     | 2.60                     | 0.60              |
| 10:C:1693:LYS:NZ    | 10:C:1749:ASP:OD1    | 2.32                     | 0.60              |
| 10:C8:1265:ARG:HH22 | 16:A8:115:SER:CB     | 2.14                     | 0.60              |
| 11:A16:302:GLN:HE22 | 11:A16:324:ARG:HH11  | 1.49                     | 0.60              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B:682:TYR:C       | 18:B:684:ILE:H      | 2.08                     | 0.60              |
| 18:B:1256:THR:HG21   | 24:D16:1238:GLU:CG  | 2.25                     | 0.60              |
| 18:B8:503:SER:N      | 18:B8:504:PRO:CD    | 2.63                     | 0.60              |
| 18:B8:1684:TRP:CH2   | 18:B8:1752:PRO:HG2  | 2.37                     | 0.60              |
| 20:E:443:ASP:O       | 20:E:445:LYS:N      | 2.35                     | 0.60              |
| 23:J32:688:PRO:O     | 23:J32:692:VAL:HG23 | 2.00                     | 0.60              |
| 23:J32:718:GLN:HE22  | 23:J32:737:TRP:HZ3  | 1.43                     | 0.60              |
| 21:H16:243:LEU:CD1   | 23:J16:603:LEU:HG   | 2.31                     | 0.60              |
| 24:D8:1328:ASN:HD21  | 24:D16:729:LEU:HD23 | 1.66                     | 0.60              |
| 24:D32:758:ALA:HB1   | 24:D32:759:TYR:CD2  | 2.36                     | 0.60              |
| 10:C32:798:VAL:CG1   | 10:C32:802:TRP:CZ2  | 2.83                     | 0.60              |
| 10:C32:1594:PRO:HB3  | 10:C32:1645:PHE:CD1 | 2.35                     | 0.60              |
| 12:A48:302:GLN:HE22  | 12:A48:324:ARG:HH11 | 1.49                     | 0.60              |
| 2:M:251:HIS:CE1      | 2:M:273:VAL:CG2     | 2.85                     | 0.60              |
| 1:R8:634:ARG:HG3     | 4:T8:160:HIS:CE1    | 2.37                     | 0.60              |
| 2:M8:251:HIS:CE1     | 2:M8:273:VAL:CG2    | 2.85                     | 0.60              |
| 2:M8:478:TRP:HA      | 2:M8:513:PRO:HG2    | 1.83                     | 0.60              |
| 5:P:633:LEU:HD21     | 5:P:647:LEU:HD11    | 1.84                     | 0.60              |
| 6:O:133:LEU:HD21     | 6:O:153:PHE:CE2     | 2.37                     | 0.60              |
| 5:P8:56:ASN:CB       | 5:P8:59:LEU:HD12    | 2.27                     | 0.60              |
| 5:P8:105:ARG:HD3     | 5:P8:130:VAL:HG22   | 1.84                     | 0.60              |
| 9:K:1232:LEU:HD23    | 9:K:1265:ILE:HG21   | 1.82                     | 0.60              |
| 10:C16:1767:LEU:HD11 | 10:C16:1832:MET:HE1 | 1.84                     | 0.60              |
| 10:C24:717:GLU:O     | 10:C24:719:PRO:N    | 2.34                     | 0.60              |
| 10:C24:1061:ASN:O    | 10:C24:1063:PRO:N   | 2.34                     | 0.60              |
| 12:A:649:LEU:HD21    | 12:A:662:PHE:HE1    | 1.66                     | 0.60              |
| 13:V:868:ARG:HH12    | 14:W:745:SER:HA     | 1.66                     | 0.60              |
| 10:C:1530:PHE:O      | 10:C:1533:THR:OG1   | 2.20                     | 0.60              |
| 10:C:1767:LEU:HD11   | 10:C:1832:MET:HE1   | 1.84                     | 0.60              |
| 10:C8:1010:ALA:HA    | 10:C8:1192:ARG:HH21 | 1.65                     | 0.60              |
| 11:A16:159:LYS:NZ    | 18:B:1918:ARG:HE    | 2.00                     | 0.60              |
| 18:B:603:PHE:CG      | 18:B:619:ARG:NH1    | 2.69                     | 0.60              |
| 18:B:1152:ASP:CG     | 18:B:1378:LYS:NZ    | 2.57                     | 0.60              |
| 18:B:1165:SER:HB2    | 18:B:1393:LEU:HD11  | 1.84                     | 0.60              |
| 18:B:1424:LEU:HD22   | 18:B:1490:ILE:HD12  | 1.83                     | 0.60              |
| 21:H16:237:PHE:HB2   | 21:H16:238:PRO:HD3  | 1.83                     | 0.60              |
| 10:C32:847:ARG:O     | 10:C32:906:ARG:NH1  | 2.34                     | 0.60              |
| 10:C32:1583:ILE:HD11 | 10:C32:1631:LYS:HB3 | 1.83                     | 0.60              |
| 1:R:1182:PRO:C       | 1:R:1184:GLU:H      | 2.10                     | 0.60              |
| 2:M:377:ARG:NH1      | 2:M:477:ASP:CG      | 2.59                     | 0.60              |
| 1:R8:1191:LYS:HB2    | 24:D40:1453:GLU:CG  | 2.32                     | 0.60              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:354:ASP:C       | 2:M8:356:GLU:H       | 2.08                     | 0.60              |
| 2:M8:385:LEU:HD11    | 2:M8:396:PHE:HE2     | 1.58                     | 0.60              |
| 2:M8:614:TYR:CE2     | 2:M8:618:HIS:HE1     | 2.20                     | 0.60              |
| 2:M8:784:GLY:HA3     | 8:L16:472:GLU:OE2    | 2.01                     | 0.60              |
| 1:R16:1466:LYS:HG3   | 6:O16:160:LEU:HD22   | 1.82                     | 0.60              |
| 6:O:23:ARG:HG2       | 6:O:37:GLU:HG2       | 1.84                     | 0.60              |
| 5:P8:663:LEU:HB2     | 5:P8:707:ASN:ND2     | 2.14                     | 0.60              |
| 5:P16:47:ASN:OD1     | 5:P16:471:SER:CB     | 2.50                     | 0.60              |
| 6:O16:173:VAL:CG2    | 6:O16:189:LEU:HD13   | 2.27                     | 0.60              |
| 8:L16:1034:VAL:CG2   | 8:L16:1068:PHE:CE2   | 2.70                     | 0.60              |
| 10:C16:1061:ASN:O    | 10:C16:1063:PRO:N    | 2.34                     | 0.60              |
| 10:C16:1726:PRO:O    | 21:H:275:LYS:HB2     | 2.02                     | 0.60              |
| 11:A40:468:VAL:HG21  | 24:D32:1103:LEU:HD12 | 1.76                     | 0.60              |
| 10:C:962:PHE:CZ      | 10:C:997:ILE:HD12    | 2.36                     | 0.60              |
| 10:C:1211:VAL:HG13   | 10:C:1232:ILE:HD13   | 1.82                     | 0.60              |
| 10:C8:698:PHE:CZ     | 10:C8:749:LEU:HD11   | 2.36                     | 0.60              |
| 18:B:729:LEU:CB      | 18:B:1196:MET:CE     | 2.74                     | 0.60              |
| 18:B:1684:TRP:CH2    | 18:B:1752:PRO:HG2    | 2.37                     | 0.60              |
| 18:B8:603:PHE:CG     | 18:B8:619:ARG:NH1    | 2.69                     | 0.60              |
| 20:E:414:MET:HE3     | 20:E:455:TYR:CE2     | 2.37                     | 0.60              |
| 23:J32:623:GLU:CD    | 23:J32:626:ARG:HH21  | 2.08                     | 0.60              |
| 10:C32:573:GLU:N     | 10:C32:574:PRO:CD    | 2.64                     | 0.60              |
| 2:M:166:THR:H        | 2:M:169:THR:HG1      | 1.47                     | 0.60              |
| 2:M:354:ASP:C        | 2:M:356:GLU:H        | 2.08                     | 0.60              |
| 3:N8:26:ILE:HD12     | 3:N8:40:VAL:HG21     | 1.84                     | 0.60              |
| 3:N8:97:HIS:CD2      | 3:N8:99:PHE:CE1      | 2.90                     | 0.60              |
| 2:M16:354:ASP:C      | 2:M16:356:GLU:N      | 2.60                     | 0.60              |
| 2:M16:385:LEU:CD1    | 2:M16:396:PHE:CD2    | 2.83                     | 0.60              |
| 5:P8:16:PHE:CZ       | 5:P8:461:HIS:NE2     | 2.70                     | 0.60              |
| 5:P16:214:LEU:CD2    | 5:P16:236:VAL:HG13   | 2.31                     | 0.60              |
| 9:K:722:GLN:O        | 9:K:723:ALA:C        | 2.39                     | 0.60              |
| 9:K:959:TRP:CH2      | 9:K:992:GLN:HB3      | 2.37                     | 0.60              |
| 11:A24:390:ALA:CB    | 24:D16:1099:ARG:CB   | 2.67                     | 0.60              |
| 10:C24:1010:ALA:HA   | 10:C24:1192:ARG:HH21 | 1.65                     | 0.60              |
| 10:C24:1767:LEU:HD11 | 10:C24:1832:MET:HE1  | 1.84                     | 0.60              |
| 10:C8:653:TYR:HE1    | 10:C8:679:ARG:HD3    | 1.65                     | 0.60              |
| 10:C8:1023:LEU:HA    | 10:C8:1210:ILE:HD11  | 1.84                     | 0.60              |
| 10:C8:1767:LEU:HD11  | 10:C8:1832:MET:HE1   | 1.84                     | 0.60              |
| 11:A16:288:HIS:HB2   | 11:A16:354:ARG:HH12  | 1.64                     | 0.60              |
| 11:A16:515:LEU:HB3   | 11:A16:516:PRO:HD3   | 1.84                     | 0.60              |
| 11:A16:703:ALA:HB1   | 24:D16:1398:ARG:NH1  | 2.10                     | 0.60              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:159:LYS:NZ    | 18:B8:1918:ARG:HE    | 2.00                     | 0.60              |
| 18:B:268:GLN:NE2     | 18:B:323:GLU:CB      | 2.65                     | 0.60              |
| 18:B8:1940:ALA:HB3   | 18:B8:1950:ILE:HD13  | 1.84                     | 0.60              |
| 19:4:110:GLY:HA2     | 19:4:418:LYS:HE3     | 1.84                     | 0.60              |
| 21:H:237:PHE:HB2     | 21:H:238:PRO:HD3     | 1.83                     | 0.60              |
| 21:H:253:ARG:NH2     | 23:J32:621:GLU:OE2   | 2.35                     | 0.60              |
| 21:H8:253:ARG:NH2    | 23:J8:621:GLU:OE2    | 2.35                     | 0.60              |
| 21:H16:361:ARG:NH2   | 22:I16:354:ASP:OD1   | 2.31                     | 0.60              |
| 1:R:634:ARG:CG       | 4:T:160:HIS:CE1      | 2.84                     | 0.60              |
| 2:M:246:ALA:HB1      | 2:M:290:ILE:HG12     | 1.83                     | 0.60              |
| 2:M:578:ARG:CZ       | 2:M:582:GLU:OE2      | 2.50                     | 0.60              |
| 2:M:738:ILE:HD11     | 2:M:779:SER:CB       | 2.29                     | 0.60              |
| 2:M:762:LEU:HD13     | 2:M:813:ASN:HD22     | 1.67                     | 0.60              |
| 1:R8:1182:PRO:C      | 1:R8:1184:GLU:H      | 2.10                     | 0.60              |
| 1:R8:1225:PHE:CD2    | 1:R8:1241:TYR:CE2    | 2.89                     | 0.60              |
| 1:R8:1349:ARG:HG3    | 1:R8:1390:GLU:OE2    | 2.01                     | 0.60              |
| 2:M8:593:HIS:CD2     | 3:N8:224:LEU:CD2     | 2.84                     | 0.60              |
| 5:P:505:GLU:CD       | 6:O:41:SER:HB3       | 2.27                     | 0.60              |
| 5:P:663:LEU:HB2      | 5:P:707:ASN:ND2      | 2.14                     | 0.60              |
| 5:P8:507:GLN:NE2     | 7:Q8:136:ARG:NH2     | 2.49                     | 0.60              |
| 7:Q8:295:SER:C       | 7:Q8:297:VAL:N       | 2.54                     | 0.60              |
| 8:L16:851:PRO:HG3    | 9:K16:1283:PRO:CB    | 2.19                     | 0.60              |
| 9:K8:635:ALA:O       | 9:K8:638:TRP:NE1     | 2.32                     | 0.60              |
| 10:C16:1283:LEU:O    | 10:C16:1287:MET:N    | 2.33                     | 0.60              |
| 10:C16:1615:PHE:HB3  | 10:C16:1674:LEU:HD23 | 1.84                     | 0.60              |
| 11:A24:607:ARG:NH1   | 24:D16:914:PHE:CE1   | 2.69                     | 0.60              |
| 10:C24:1614:LEU:HD11 | 10:C24:1635:LEU:CD2  | 2.32                     | 0.60              |
| 10:C24:1708:ARG:NH1  | 21:H24:276:GLY:HA2   | 2.17                     | 0.60              |
| 12:A:302:GLN:HE22    | 12:A:324:ARG:HH11    | 1.49                     | 0.60              |
| 10:C:1271:PHE:HE2    | 10:C:1284:ASP:HB3    | 1.53                     | 0.60              |
| 10:C8:1061:ASN:O     | 10:C8:1063:PRO:N     | 2.34                     | 0.60              |
| 11:A16:560:MET:CE    | 11:A16:615:GLN:CD    | 2.73                     | 0.60              |
| 11:A32:120:ALA:HB1   | 18:B8:1520:LEU:CD1   | 2.31                     | 0.60              |
| 11:A32:560:MET:CE    | 11:A32:615:GLN:CD    | 2.73                     | 0.60              |
| 18:B:771:MET:CE      | 18:B:840:VAL:HG21    | 2.32                     | 0.60              |
| 18:B:1911:LEU:CD1    | 18:B:1960:LEU:HD12   | 2.31                     | 0.60              |
| 18:B:1940:ALA:HB3    | 18:B:1950:ILE:HD13   | 1.84                     | 0.60              |
| 18:B8:32:LEU:CD2     | 18:B8:36:ILE:CG2     | 2.80                     | 0.60              |
| 19:4:329:SER:OG      | 19:4:333:SER:CB      | 2.50                     | 0.60              |
| 20:E:352:PHE:CD1     | 20:E:451:ILE:CD1     | 2.78                     | 0.60              |
| 22:I:203:GLN:N       | 22:I:204:PRO:CD      | 2.64                     | 0.60              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 21:H24:287:ILE:HG23  | 22:I24:273:LEU:CD1  | 2.31                     | 0.60              |
| 22:I24:203:GLN:N     | 22:I24:204:PRO:CD   | 2.64                     | 0.60              |
| 24:D40:758:ALA:HB1   | 24:D40:759:TYR:CD2  | 2.36                     | 0.60              |
| 10:C32:1111:SER:C    | 10:C32:1113:LYS:N   | 2.58                     | 0.60              |
| 10:C32:1290:HIS:HD2  | 10:C32:1334:MET:HE2 | 1.66                     | 0.60              |
| 10:C32:1465:LEU:O    | 10:C32:1469:HIS:ND1 | 2.34                     | 0.60              |
| 10:C32:1693:LYS:NZ   | 10:C32:1749:ASP:OD1 | 2.32                     | 0.60              |
| 12:A48:212:LYS:NZ    | 12:A48:585:MET:HE3  | 2.16                     | 0.60              |
| 1:R:1115:TYR:CB      | 1:R:1131:MET:HE3    | 2.32                     | 0.59              |
| 1:R:1139:ARG:HB2     | 1:R:1157:ARG:NH2    | 2.18                     | 0.59              |
| 1:R:1324:ASP:OD1     | 10:C:1180:ILE:HG21  | 1.97                     | 0.59              |
| 2:M:417:ARG:HB3      | 8:L:346:TRP:CE2     | 2.37                     | 0.59              |
| 2:M16:614:TYR:CE2    | 2:M16:618:HIS:HE1   | 2.20                     | 0.59              |
| 5:P:247:GLU:OE1      | 5:P:296:PHE:N       | 2.29                     | 0.59              |
| 7:Q:200:PHE:CZ       | 7:Q:228:ALA:HA      | 2.37                     | 0.59              |
| 5:P16:30:TYR:CE2     | 5:P16:32:LEU:HB2    | 2.36                     | 0.59              |
| 10:C16:1547:LYS:CE   | 24:D8:1405:GLY:CA   | 2.80                     | 0.59              |
| 11:A40:515:LEU:HB3   | 11:A40:516:PRO:HD3  | 1.84                     | 0.59              |
| 10:C:847:ARG:O       | 10:C:906:ARG:NH1    | 2.34                     | 0.59              |
| 11:A16:36:ASN:ND2    | 22:I:293:LYS:HZ1    | 1.91                     | 0.59              |
| 20:E:437:SER:O       | 20:E:439:MET:N      | 2.34                     | 0.59              |
| 19:48:55:GLN:C       | 19:48:57:ASN:H      | 2.09                     | 0.59              |
| 20:E8:38:PHE:O       | 20:E8:39:SER:C      | 2.41                     | 0.59              |
| 20:E8:414:MET:HE3    | 20:E8:455:TYR:CE2   | 2.37                     | 0.59              |
| 21:H:301:ARG:HH21    | 22:I:284:GLU:CD     | 2.10                     | 0.59              |
| 21:H8:361:ARG:NH2    | 22:I8:354:ASP:OD1   | 2.32                     | 0.59              |
| 21:H24:255:LEU:HD12  | 23:J24:655:GLU:CD   | 2.22                     | 0.59              |
| 24:D8:857:THR:HG21   | 24:D8:885:TYR:HH    | 1.52                     | 0.59              |
| 10:C32:1767:LEU:HD11 | 10:C32:1832:MET:HE1 | 1.84                     | 0.59              |
| 1:R:1362:ASP:N       | 10:C:608:ASP:OD2    | 2.34                     | 0.59              |
| 1:R:1428:VAL:CG2     | 6:O:165:LYS:HZ2     | 2.11                     | 0.59              |
| 2:M16:349:ASP:C      | 2:M16:351:ALA:H     | 2.09                     | 0.59              |
| 5:P8:394:ASN:O       | 5:P8:396:SER:N      | 2.29                     | 0.59              |
| 5:P16:16:PHE:CZ      | 5:P16:461:HIS:NE2   | 2.70                     | 0.59              |
| 5:P16:303:LYS:HB3    | 5:P16:304:PRO:HD3   | 1.84                     | 0.59              |
| 5:P16:507:GLN:NE2    | 7:Q16:136:ARG:NH2   | 2.49                     | 0.59              |
| 5:P16:607:PHE:HB3    | 5:P16:629:ARG:NH1   | 2.17                     | 0.59              |
| 9:K:911:LEU:HB3      | 9:K:945:LEU:HD11    | 1.84                     | 0.59              |
| 9:K:1048:GLN:HE22    | 9:K:1128:ARG:HG2    | 1.64                     | 0.59              |
| 9:K8:842:ILE:HG23    | 9:K8:871:LEU:HD21   | 1.82                     | 0.59              |
| 9:K8:955:TYR:CE1     | 9:K8:985:PHE:CA     | 2.85                     | 0.59              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1010:ALA:HA   | 10:C16:1192:ARG:HH21 | 1.65                     | 0.59              |
| 10:C16:1265:ARG:HH22 | 11:A24:115:SER:CB    | 2.15                     | 0.59              |
| 10:C24:453:LEU:HB3   | 10:C24:459:LEU:HD22  | 1.85                     | 0.59              |
| 10:C24:667:ILE:CG2   | 10:C24:670:GLU:N     | 2.59                     | 0.59              |
| 10:C24:966:CYS:HA    | 10:C24:1025:LEU:HD12 | 1.83                     | 0.59              |
| 11:A40:694:GLU:CD    | 24:D24:1398:ARG:HA   | 2.26                     | 0.59              |
| 11:A16:91:GLU:HB2    | 18:B:1112:LYS:HZ1    | 1.58                     | 0.59              |
| 18:B:334:PHE:CE1     | 18:B:338:ILE:CD1     | 2.85                     | 0.59              |
| 18:B8:268:GLN:NE2    | 18:B8:323:GLU:CB     | 2.65                     | 0.59              |
| 18:B8:1165:SER:HB2   | 18:B8:1393:LEU:HD11  | 1.84                     | 0.59              |
| 18:B8:1911:LEU:CD1   | 18:B8:1960:LEU:HD12  | 2.31                     | 0.59              |
| 20:E:437:SER:C       | 20:E:439:MET:N       | 2.52                     | 0.59              |
| 21:H:240:ILE:HD13    | 22:I:174:GLN:OE1     | 2.02                     | 0.59              |
| 21:H8:244:ARG:NH2    | 22:I8:177:VAL:CG1    | 2.65                     | 0.59              |
| 21:H24:244:ARG:NH2   | 22:I24:177:VAL:CG1   | 2.65                     | 0.59              |
| 24:D:308:ASN:HD22    | 24:D16:753:ARG:CD    | 2.15                     | 0.59              |
| 1:R:1459:ARG:HG2     | 10:C:731:GLN:HE22    | 1.67                     | 0.59              |
| 2:M:478:TRP:HA       | 2:M:513:PRO:HG2      | 1.83                     | 0.59              |
| 2:M:762:LEU:HD13     | 2:M:813:ASN:ND2      | 2.17                     | 0.59              |
| 1:R8:1249:SER:HB2    | 1:R8:1280:GLU:OE2    | 2.02                     | 0.59              |
| 2:M16:278:VAL:HG11   | 2:M16:326:GLN:HG3    | 1.84                     | 0.59              |
| 5:P:97:SER:HB3       | 5:P:98:PRO:HD3       | 1.82                     | 0.59              |
| 5:P8:10:GLY:HA2      | 5:P8:26:TYR:OH       | 2.02                     | 0.59              |
| 6:O8:133:LEU:HD21    | 6:O8:153:PHE:CE2     | 2.37                     | 0.59              |
| 5:P16:425:TRP:CD1    | 5:P16:465:TYR:HH     | 2.18                     | 0.59              |
| 8:L16:1074:ARG:HH11  | 9:K16:1089:LYS:HD2   | 1.67                     | 0.59              |
| 10:C16:8:VAL:HG23    | 10:C16:129:ASP:O     | 2.02                     | 0.59              |
| 10:C16:453:LEU:HB3   | 10:C16:459:LEU:HD22  | 1.85                     | 0.59              |
| 10:C16:1614:LEU:HD11 | 10:C16:1635:LEU:CD2  | 2.32                     | 0.59              |
| 11:A24:515:LEU:HB3   | 11:A24:516:PRO:HD3   | 1.84                     | 0.59              |
| 12:A:642:GLY:HA2     | 12:A:685:ARG:NE      | 2.16                     | 0.59              |
| 10:C:1283:LEU:O      | 10:C:1287:MET:N      | 2.33                     | 0.59              |
| 10:C:1583:ILE:HD11   | 10:C:1631:LYS:HB3    | 1.83                     | 0.59              |
| 10:C8:582:GLU:HG3    | 10:C8:637:TYR:CE2    | 2.38                     | 0.59              |
| 10:C8:1583:ILE:HD11  | 10:C8:1631:LYS:HB3   | 1.83                     | 0.59              |
| 18:B:32:LEU:CD2      | 18:B:36:ILE:CG2      | 2.80                     | 0.59              |
| 18:B:50:THR:HG21     | 18:B:179:GLN:HE22    | 1.63                     | 0.59              |
| 18:B:536:ILE:HG21    | 18:B:545:VAL:HG11    | 1.83                     | 0.59              |
| 18:B:968:PHE:CZ      | 18:B:998:LEU:HD23    | 2.37                     | 0.59              |
| 18:B:1122:SER:C      | 18:B:1124:GLY:H      | 2.10                     | 0.59              |
| 18:B8:334:PHE:CE1    | 18:B8:338:ILE:CD1    | 2.85                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B8:618:VAL:CG1   | 18:B8:621:VAL:CG2   | 2.75                     | 0.59              |
| 19:48:250:ILE:HD11  | 20:E8:163:ILE:CD1   | 2.22                     | 0.59              |
| 19:48:329:SER:OG    | 19:48:333:SER:CB    | 2.50                     | 0.59              |
| 20:E8:352:PHE:CD1   | 20:E8:451:ILE:CD1   | 2.78                     | 0.59              |
| 21:H:366:MET:HE1    | 22:I:332:MET:HE2    | 1.83                     | 0.59              |
| 21:H8:240:ILE:HD13  | 22:I8:174:GLN:OE1   | 2.02                     | 0.59              |
| 21:H8:363:MET:SD    | 22:I8:332:MET:CE    | 2.81                     | 0.59              |
| 22:I8:96:PHE:CE2    | 22:I8:113:HIS:CG    | 2.91                     | 0.59              |
| 21:H24:253:ARG:NH2  | 23:J24:621:GLU:OE2  | 2.35                     | 0.59              |
| 21:H16:240:ILE:HD13 | 22:I16:174:GLN:OE1  | 2.02                     | 0.59              |
| 21:H16:253:ARG:NH2  | 23:J16:621:GLU:OE2  | 2.35                     | 0.59              |
| 12:A48:259:ILE:CG2  | 12:A48:276:LEU:CD2  | 2.80                     | 0.59              |
| 2:M:641:CYS:SG      | 2:M:668:LEU:HD23    | 2.42                     | 0.59              |
| 1:R8:1059:ILE:HD13  | 24:D40:1435:ARG:NH2 | 2.18                     | 0.59              |
| 2:M8:377:ARG:NH1    | 2:M8:477:ASP:CG     | 2.59                     | 0.59              |
| 2:M8:385:LEU:CD1    | 2:M8:396:PHE:CD2    | 2.83                     | 0.59              |
| 2:M8:641:CYS:SG     | 2:M8:668:LEU:HD23   | 2.42                     | 0.59              |
| 2:M16:339:GLU:OE2   | 4:T8:638:SER:O      | 2.21                     | 0.59              |
| 2:M16:478:TRP:HA    | 2:M16:513:PRO:HG2   | 1.83                     | 0.59              |
| 2:M16:578:ARG:CZ    | 2:M16:582:GLU:OE2   | 2.50                     | 0.59              |
| 3:N16:26:ILE:HD12   | 3:N16:40:VAL:HG21   | 1.84                     | 0.59              |
| 5:P:109:ILE:HD13    | 14:W:18:PRO:HB2     | 1.84                     | 0.59              |
| 5:P8:505:GLU:CD     | 6:O8:41:SER:HB3     | 2.27                     | 0.59              |
| 5:P8:610:SER:C      | 5:P8:629:ARG:NH2    | 2.57                     | 0.59              |
| 5:P16:247:GLU:OE1   | 5:P16:295:LYS:HA    | 2.03                     | 0.59              |
| 5:P16:505:GLU:CD    | 6:O16:41:SER:HB3    | 2.27                     | 0.59              |
| 8:L8:598:LEU:HD23   | 8:L8:627:ARG:NH1    | 2.16                     | 0.59              |
| 8:L8:1077:LEU:HD13  | 9:K8:1086:VAL:HG11  | 1.77                     | 0.59              |
| 9:K:1214:TYR:HB2    | 9:K:1269:CYS:SG     | 2.42                     | 0.59              |
| 10:C24:8:VAL:HG23   | 10:C24:129:ASP:O    | 2.02                     | 0.59              |
| 10:C24:16:LEU:CD2   | 10:C24:139:ARG:NH1  | 2.66                     | 0.59              |
| 10:C24:123:TRP:CH2  | 10:C24:127:ARG:HD2  | 2.37                     | 0.59              |
| 10:C24:919:ASP:H    | 10:C24:927:THR:CG2  | 2.16                     | 0.59              |
| 10:C24:1699:LYS:NZ  | 23:J24:722:LEU:HD21 | 2.11                     | 0.59              |
| 12:A:437:LEU:CD1    | 12:A:454:LYS:HZ3    | 2.16                     | 0.59              |
| 13:V:804:VAL:HG13   | 14:W:695:LEU:HD11   | 1.84                     | 0.59              |
| 13:V:835:GLU:HG2    | 15:J:648:TYR:HH     | 1.67                     | 0.59              |
| 10:C:275:ALA:HB1    | 10:C:326:LEU:HD12   | 1.82                     | 0.59              |
| 10:C:979:MET:HE2    | 10:C:1028:ILE:HG21  | 1.82                     | 0.59              |
| 10:C:1023:LEU:HA    | 10:C:1210:ILE:HD11  | 1.84                     | 0.59              |
| 10:C8:1615:PHE:HB3  | 10:C8:1674:LEU:HD23 | 1.84                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A32:212:LYS:NZ   | 11:A32:585:MET:HE1  | 2.09                     | 0.59              |
| 18:B:286:GLN:OE1    | 18:B:443:PHE:CD1    | 2.56                     | 0.59              |
| 18:B:1129:LYS:O     | 18:B:1131:THR:N     | 2.34                     | 0.59              |
| 18:B:1264:GLN:HE22  | 18:B:1394:TRP:HZ3   | 1.50                     | 0.59              |
| 18:B8:286:GLN:OE1   | 18:B8:443:PHE:CD1   | 2.56                     | 0.59              |
| 18:B8:968:PHE:CZ    | 18:B8:998:LEU:HD23  | 2.37                     | 0.59              |
| 18:B8:1122:SER:C    | 18:B8:1124:GLY:H    | 2.09                     | 0.59              |
| 18:B8:1856:PHE:CD1  | 18:B8:1857:PRO:HD2  | 2.36                     | 0.59              |
| 19:4:55:GLN:C       | 19:4:57:ASN:N       | 2.60                     | 0.59              |
| 21:H8:287:ILE:HG23  | 22:I8:273:LEU:CD1   | 2.31                     | 0.59              |
| 22:I24:96:PHE:CE2   | 22:I24:113:HIS:CG   | 2.91                     | 0.59              |
| 24:D:308:ASN:ND2    | 24:D16:753:ARG:CG   | 2.65                     | 0.59              |
| 24:D32:764:GLU:OE1  | 24:D40:620:GLN:NE2  | 2.36                     | 0.59              |
| 24:D40:839:GLU:CA   | 24:D40:971:HIS:CE1  | 2.85                     | 0.59              |
| 12:A48:515:LEU:HB3  | 12:A48:516:PRO:HD3  | 1.84                     | 0.59              |
| 1:R:1334:GLU:HB3    | 10:C:1170:VAL:HG23  | 1.84                     | 0.59              |
| 3:N:26:ILE:HD12     | 3:N:40:VAL:HG21     | 1.84                     | 0.59              |
| 1:R8:1115:TYR:CB    | 1:R8:1131:MET:HE3   | 2.32                     | 0.59              |
| 2:M16:540:TYR:HD1   | 2:M16:555:LEU:HD21  | 1.38                     | 0.59              |
| 5:P:247:GLU:OE1     | 5:P:295:LYS:HA      | 2.03                     | 0.59              |
| 5:P8:214:LEU:CD2    | 5:P8:236:VAL:HG13   | 2.31                     | 0.59              |
| 5:P8:451:LYS:CD     | 6:O8:312:ASN:O      | 2.50                     | 0.59              |
| 9:K8:1074:ARG:NE    | 9:K8:1126:LEU:HD22  | 2.16                     | 0.59              |
| 10:C16:16:LEU:CD2   | 10:C16:139:ARG:NH1  | 2.66                     | 0.59              |
| 10:C16:1530:PHE:O   | 10:C16:1533:THR:OG1 | 2.20                     | 0.59              |
| 10:C24:275:ALA:HB1  | 10:C24:326:LEU:HD12 | 1.83                     | 0.59              |
| 10:C24:768:ARG:CZ   | 10:C24:775:LYS:CG   | 2.69                     | 0.59              |
| 10:C24:1111:SER:C   | 10:C24:1113:LYS:N   | 2.58                     | 0.59              |
| 10:C:16:LEU:CD2     | 10:C:139:ARG:NH1    | 2.66                     | 0.59              |
| 10:C:667:ILE:CG2    | 10:C:669:GLY:C      | 2.68                     | 0.59              |
| 10:C:1615:PHE:HB3   | 10:C:1674:LEU:HD23  | 1.84                     | 0.59              |
| 10:C:1805:ASP:OD1   | 10:C:1830:LYS:NZ    | 2.27                     | 0.59              |
| 10:C8:123:TRP:CH2   | 10:C8:127:ARG:HD2   | 2.36                     | 0.59              |
| 10:C8:1614:LEU:HD11 | 10:C8:1635:LEU:CD2  | 2.32                     | 0.59              |
| 11:A16:90:PHE:CD1   | 18:B:1788:ILE:HG22  | 2.28                     | 0.59              |
| 18:B:202:LEU:CD1    | 18:B:820:ARG:HH11   | 2.15                     | 0.59              |
| 18:B:235:ARG:NH1    | 18:B:308:GLU:CD     | 2.55                     | 0.59              |
| 18:B:1205:ILE:CD1   | 18:B:1271:PHE:CE2   | 2.85                     | 0.59              |
| 18:B8:684:ILE:HD11  | 24:D32:1065:ALA:HB3 | 1.84                     | 0.59              |
| 18:B8:771:MET:CE    | 18:B8:840:VAL:HG21  | 2.32                     | 0.59              |
| 18:B8:938:LEU:HD11  | 18:B8:1005:TYR:CZ   | 2.37                     | 0.59              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B8:1205:ILE:CD1  | 18:B8:1271:PHE:CE2   | 2.85                     | 0.59              |
| 20:E:40:THR:HG22    | 20:E:125:SER:HB2     | 1.85                     | 0.59              |
| 20:E:433:LYS:C      | 20:E:435:ALA:H       | 2.02                     | 0.59              |
| 19:48:178:ASN:OD1   | 20:E8:416:LYS:HE2    | 2.03                     | 0.59              |
| 19:48:306:ASP:OD1   | 19:48:307:PRO:CD     | 2.49                     | 0.59              |
| 20:E8:40:THR:HG22   | 20:E8:125:SER:HB2    | 1.85                     | 0.59              |
| 21:H:255:LEU:HD12   | 23:J32:655:GLU:CD    | 2.23                     | 0.59              |
| 22:I16:289:LEU:HD23 | 22:I16:296:ARG:NH2   | 2.10                     | 0.59              |
| 12:A48:388:VAL:HG12 | 12:A48:392:SER:HB2   | 1.85                     | 0.59              |
| 1:R:1449:TRP:CE3    | 2:M:160:LEU:CD1      | 2.81                     | 0.59              |
| 2:M:552:PHE:HZ      | 2:M:559:PHE:CE2      | 2.17                     | 0.59              |
| 1:R8:1059:ILE:HD13  | 24:D40:1435:ARG:HH21 | 1.66                     | 0.59              |
| 2:M8:354:ASP:C      | 2:M8:356:GLU:N       | 2.60                     | 0.59              |
| 2:M8:417:ARG:HH21   | 8:L8:415:PHE:HE2     | 1.45                     | 0.59              |
| 1:R16:1182:PRO:C    | 1:R16:1184:GLU:H     | 2.10                     | 0.59              |
| 5:P:620:ILE:HG23    | 5:P:660:ARG:HH21     | 1.68                     | 0.59              |
| 5:P16:157:SER:O     | 5:P16:251:LYS:NZ     | 2.22                     | 0.59              |
| 5:P16:620:ILE:CG2   | 5:P16:660:ARG:NH2    | 2.66                     | 0.59              |
| 8:L:1069:LEU:HD21   | 9:K:1086:VAL:HG21    | 1.85                     | 0.59              |
| 8:L8:179:VAL:CG2    | 10:C32:1360:GLN:HG2  | 2.33                     | 0.59              |
| 9:K8:911:LEU:HB3    | 9:K8:945:LEU:HD11    | 1.84                     | 0.59              |
| 14:W:711:ARG:CG     | 10:C8:1609:ASP:OD2   | 2.50                     | 0.59              |
| 10:C:619:LEU:CB     | 10:C:620:PRO:CD      | 2.79                     | 0.59              |
| 10:C:1519:ARG:NH2   | 10:C:1578:LEU:HB2    | 2.18                     | 0.59              |
| 10:C8:919:ASP:H     | 10:C8:927:THR:CG2    | 2.16                     | 0.59              |
| 11:A16:388:VAL:HG12 | 11:A16:392:SER:HB2   | 1.85                     | 0.59              |
| 11:A16:437:LEU:CD1  | 11:A16:454:LYS:NZ    | 2.66                     | 0.59              |
| 18:B:671:MET:HE1    | 18:B:736:ALA:HB2     | 1.84                     | 0.59              |
| 18:B8:235:ARG:NH1   | 18:B8:308:GLU:CD     | 2.55                     | 0.59              |
| 18:B8:1058:ILE:HG23 | 18:B8:1154:ILE:HD11  | 1.85                     | 0.59              |
| 18:B8:1505:MET:HE3  | 18:B8:1518:VAL:HG21  | 1.82                     | 0.59              |
| 20:E8:350:GLU:HB3   | 20:E8:352:PHE:HD2    | 1.67                     | 0.59              |
| 22:I24:210:LYS:C    | 22:I16:139:GLN:NE2   | 2.61                     | 0.59              |
| 10:C32:743:PHE:CE2  | 10:C32:749:LEU:CD2   | 2.86                     | 0.59              |
| 10:C32:1615:PHE:HB3 | 10:C32:1674:LEU:HD23 | 1.84                     | 0.59              |
| 10:C32:1660:SER:C   | 10:C32:1662:ASP:N    | 2.59                     | 0.59              |
| 12:A48:590:TYR:CD2  | 12:A48:623:LEU:HB3   | 2.38                     | 0.59              |
| 1:R:1188:TYR:CZ     | 24:D:1459:LEU:CB     | 2.86                     | 0.59              |
| 2:M:217:ILE:CD1     | 3:N:8:THR:HG21       | 2.33                     | 0.59              |
| 1:R8:1269:LEU:HB3   | 5:P8:684:ARG:HG2     | 1.85                     | 0.59              |
| 2:M8:762:LEU:HD13   | 2:M8:813:ASN:HD22    | 1.68                     | 0.59              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R16:1139:ARG:CB   | 1:R16:1157:ARG:CZ    | 2.79                     | 0.59              |
| 5:P:96:VAL:CG1      | 5:P:481:ILE:HD13     | 2.31                     | 0.59              |
| 5:P8:12:GLU:C       | 5:P8:14:VAL:N        | 2.60                     | 0.59              |
| 9:K:1142:ARG:NH2    | 9:K:1204:THR:CA      | 2.56                     | 0.59              |
| 9:K8:1232:LEU:HD23  | 9:K8:1265:ILE:HG21   | 1.82                     | 0.59              |
| 10:C16:966:CYS:HA   | 10:C16:1025:LEU:HD12 | 1.83                     | 0.59              |
| 10:C16:1318:ARG:HD3 | 10:C16:1398:PHE:CD1  | 2.37                     | 0.59              |
| 11:A24:590:TYR:CD2  | 11:A24:623:LEU:HB3   | 2.38                     | 0.59              |
| 10:C24:619:LEU:CB   | 10:C24:620:PRO:CD    | 2.79                     | 0.59              |
| 12:A:515:LEU:HB3    | 12:A:516:PRO:HD3     | 1.84                     | 0.59              |
| 14:W:659:ARG:NH2    | 15:J:583:LEU:CD2     | 2.53                     | 0.59              |
| 14:W:715:ASP:C      | 10:C8:1568:ARG:NH1   | 2.61                     | 0.59              |
| 10:C:743:PHE:CE2    | 10:C:749:LEU:CD2     | 2.86                     | 0.59              |
| 10:C:1234:ASP:CG    | 10:C:1302:LYS:HZ2    | 2.09                     | 0.59              |
| 10:C8:847:ARG:O     | 10:C8:906:ARG:NH1    | 2.34                     | 0.59              |
| 10:C8:1002:LEU:CD2  | 10:C8:1012:ARG:CZ    | 2.79                     | 0.59              |
| 10:C8:1519:ARG:NH2  | 10:C8:1578:LEU:HB2   | 2.18                     | 0.59              |
| 11:A32:388:VAL:HG12 | 11:A32:392:SER:HB2   | 1.85                     | 0.59              |
| 18:B8:729:LEU:CB    | 18:B8:1196:MET:CE    | 2.74                     | 0.59              |
| 19:4:304:ILE:CD1    | 19:4:359:ALA:HA      | 2.33                     | 0.59              |
| 19:48:244:GLN:NE2   | 20:E8:364:PHE:CD1    | 2.70                     | 0.59              |
| 20:E8:443:ASP:O     | 20:E8:445:LYS:N      | 2.35                     | 0.59              |
| 22:I24:196:VAL:CA   | 23:J24:620:MET:CE    | 2.46                     | 0.59              |
| 23:J24:623:GLU:CD   | 23:J24:626:ARG:HH21  | 2.08                     | 0.59              |
| 10:C32:8:VAL:HG23   | 10:C32:129:ASP:O     | 2.02                     | 0.59              |
| 10:C32:453:LEU:HB3  | 10:C32:459:LEU:HD22  | 1.85                     | 0.59              |
| 10:C32:919:ASP:H    | 10:C32:927:THR:CG2   | 2.16                     | 0.59              |
| 10:C32:1234:ASP:CG  | 10:C32:1302:LYS:HZ2  | 2.10                     | 0.59              |
| 10:C32:1318:ARG:HD3 | 10:C32:1398:PHE:CD1  | 2.37                     | 0.59              |
| 1:R:1033:LYS:HE2    | 24:D:1432:THR:HB     | 1.85                     | 0.59              |
| 1:R:1326:GLY:N      | 10:C:1154:TRP:NE1    | 2.51                     | 0.59              |
| 1:R:1330:ALA:CB     | 10:C:1173:LEU:CD1    | 2.69                     | 0.59              |
| 1:R:1349:ARG:HG3    | 1:R:1390:GLU:OE2     | 2.01                     | 0.59              |
| 2:M8:417:ARG:HB2    | 8:L8:298:PHE:CE2     | 2.31                     | 0.59              |
| 2:M16:211:MET:HE1   | 3:N16:280:ASN:HA     | 1.85                     | 0.59              |
| 2:M16:251:HIS:CE1   | 2:M16:273:VAL:CG2    | 2.85                     | 0.59              |
| 2:M16:762:LEU:HD13  | 2:M16:813:ASN:HD22   | 1.67                     | 0.59              |
| 5:P8:614:VAL:CA     | 5:P8:629:ARG:NH1     | 2.66                     | 0.59              |
| 5:P8:645:LEU:HB3    | 5:P8:646:PRO:HD3     | 1.85                     | 0.59              |
| 5:P16:10:GLY:HA2    | 5:P16:26:TYR:OH      | 2.02                     | 0.59              |
| 7:Q16:221:TRP:CD1   | 7:Q16:221:TRP:H      | 2.20                     | 0.59              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:842:ILE:CG2      | 9:K:871:LEU:HD21     | 2.33                     | 0.59              |
| 9:K8:955:TYR:CZ      | 9:K8:984:GLY:C       | 2.81                     | 0.59              |
| 10:C16:743:PHE:CE2   | 10:C16:749:LEU:CD2   | 2.86                     | 0.59              |
| 10:C16:919:ASP:H     | 10:C16:927:THR:CG2   | 2.16                     | 0.59              |
| 10:C16:1547:LYS:NZ   | 24:D8:1405:GLY:C     | 2.61                     | 0.59              |
| 10:C16:1693:LYS:NZ   | 10:C16:1749:ASP:OD1  | 2.33                     | 0.59              |
| 10:C24:386:ASN:CA    | 10:C24:449:GLU:OE1   | 2.51                     | 0.59              |
| 10:C24:743:PHE:CE2   | 10:C24:749:LEU:CD2   | 2.86                     | 0.59              |
| 10:C24:1265:ARG:HH22 | 11:A40:115:SER:CB    | 2.15                     | 0.59              |
| 11:A40:302:GLN:HE22  | 11:A40:324:ARG:HH11  | 1.49                     | 0.59              |
| 11:A40:557:LEU:HD23  | 11:A40:561:ASP:HB3   | 1.85                     | 0.59              |
| 12:A:437:LEU:CD1     | 12:A:454:LYS:NZ      | 2.66                     | 0.59              |
| 10:C:582:GLU:HG3     | 10:C:637:TYR:CE2     | 2.38                     | 0.59              |
| 18:B:457:SER:CA      | 18:B:548:ARG:HH11    | 2.14                     | 0.59              |
| 18:B:938:LEU:HD11    | 18:B:1005:TYR:CZ     | 2.37                     | 0.59              |
| 18:B8:202:LEU:CD1    | 18:B8:820:ARG:HH11   | 2.15                     | 0.59              |
| 18:B8:664:LEU:HD11   | 18:B8:729:LEU:CD2    | 2.28                     | 0.59              |
| 20:E:408:LEU:CD1     | 20:E:507:LEU:HD23    | 2.32                     | 0.59              |
| 20:E:418:THR:C       | 20:E:420:LEU:H       | 2.11                     | 0.59              |
| 19:48:419:PHE:HE2    | 19:48:424:LEU:HD11   | 1.68                     | 0.59              |
| 20:E8:347:PRO:C      | 20:E8:349:THR:H      | 2.11                     | 0.59              |
| 21:H16:244:ARG:NH2   | 22:I16:177:VAL:CG1   | 2.65                     | 0.59              |
| 10:C32:1009:GLN:C    | 10:C32:1192:ARG:NH2  | 2.60                     | 0.59              |
| 10:C32:1023:LEU:HA   | 10:C32:1210:ILE:HD11 | 1.84                     | 0.59              |
| 10:C32:1265:ARG:HH22 | 12:A48:115:SER:CB    | 2.14                     | 0.59              |
| 10:C32:1283:LEU:O    | 10:C32:1287:MET:N    | 2.33                     | 0.59              |
| 1:R:1422:SER:CB      | 6:O:154:GLN:NE2      | 2.66                     | 0.59              |
| 2:M:278:VAL:HG11     | 2:M:326:GLN:HG3      | 1.84                     | 0.59              |
| 2:M:421:LEU:HD11     | 8:L:346:TRP:NE1      | 2.17                     | 0.59              |
| 1:R16:1428:VAL:HG13  | 1:R16:1431:ARG:NE    | 2.18                     | 0.59              |
| 2:M16:217:ILE:CD1    | 3:N16:8:THR:HG21     | 2.33                     | 0.59              |
| 2:M16:627:TYR:CD1    | 3:N16:167:LEU:HA     | 2.38                     | 0.59              |
| 5:P:645:LEU:HB3      | 5:P:646:PRO:HD3      | 1.85                     | 0.59              |
| 5:P8:620:ILE:HG23    | 5:P8:660:ARG:HH21    | 1.68                     | 0.59              |
| 9:K:1074:ARG:NE      | 9:K:1126:LEU:HD22    | 2.16                     | 0.59              |
| 9:K8:840:TRP:CE3     | 9:K8:907:ILE:HD11    | 2.33                     | 0.59              |
| 11:A24:740:LEU:HD11  | 24:D16:703:SER:OG    | 2.02                     | 0.59              |
| 10:C24:510:TRP:N     | 10:C24:511:PRO:CD    | 2.66                     | 0.59              |
| 10:C24:1616:ILE:C    | 10:C24:1618:SER:H    | 2.11                     | 0.59              |
| 10:C24:1814:LYS:HZ1  | 23:J24:738:MET:HB3   | 0.59                     | 0.59              |
| 13:V:897:SER:O       | 13:V:901:THR:OG1     | 2.20                     | 0.59              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 14:W:645:HIS:ND1     | 14:W:649:LEU:CD1     | 2.58                     | 0.59              |
| 10:C:1708:ARG:HA     | 10:C:1730:ILE:HD11   | 1.85                     | 0.59              |
| 10:C:1807:LEU:HD23   | 10:C:1810:LEU:HD11   | 1.85                     | 0.59              |
| 11:A32:326:TYR:CD1   | 17:F24:77:TYR:HB3    | 2.13                     | 0.59              |
| 11:A32:590:TYR:CD2   | 11:A32:623:LEU:HB3   | 2.38                     | 0.59              |
| 18:B:282:GLU:HG3     | 18:B:444:VAL:HG21    | 1.84                     | 0.59              |
| 21:H:363:MET:HA      | 21:H:366:MET:HE3     | 1.85                     | 0.59              |
| 21:H24:366:MET:HE1   | 22:I24:332:MET:HE2   | 1.83                     | 0.59              |
| 22:I24:182:MET:CE    | 23:J24:605:LEU:HD23  | 2.33                     | 0.59              |
| 22:I16:96:PHE:CE2    | 22:I16:113:HIS:CG    | 2.91                     | 0.59              |
| 22:I16:182:MET:HE1   | 23:J16:605:LEU:HD23  | 1.85                     | 0.59              |
| 24:D8:1330:ARG:NH1   | 24:D16:719:ARG:HB3   | 2.16                     | 0.59              |
| 10:C32:16:LEU:CD2    | 10:C32:139:ARG:NH1   | 2.66                     | 0.59              |
| 2:M8:343:MET:C       | 2:M8:345:ASP:N       | 2.56                     | 0.59              |
| 2:M8:762:LEU:HD13    | 2:M8:813:ASN:ND2     | 2.17                     | 0.59              |
| 2:M16:762:LEU:HD13   | 2:M16:813:ASN:ND2    | 2.17                     | 0.59              |
| 5:P:214:LEU:CD2      | 5:P:236:VAL:HG13     | 2.31                     | 0.59              |
| 5:P:620:ILE:CG2      | 5:P:660:ARG:NH2      | 2.66                     | 0.59              |
| 5:P8:187:TRP:CZ3     | 5:P8:191:ARG:HD3     | 2.38                     | 0.59              |
| 6:O8:23:ARG:HG2      | 6:O8:37:GLU:HG2      | 1.84                     | 0.59              |
| 8:L8:608:PHE:HZ      | 8:L8:635:MET:O       | 1.85                     | 0.59              |
| 9:K:1019:ARG:NE      | 9:K:1059:ARG:CD      | 2.55                     | 0.59              |
| 10:C16:275:ALA:HB1   | 10:C16:326:LEU:HD12  | 1.83                     | 0.59              |
| 10:C16:510:TRP:N     | 10:C16:511:PRO:CD    | 2.66                     | 0.59              |
| 10:C16:653:TYR:N     | 10:C16:654:PRO:CD    | 2.66                     | 0.59              |
| 10:C16:1535:LEU:HB3  | 10:C16:1548:ILE:HD13 | 1.85                     | 0.59              |
| 10:C24:847:ARG:O     | 10:C24:906:ARG:NH1   | 2.34                     | 0.59              |
| 10:C24:1708:ARG:HG3  | 10:C24:1730:ILE:CD1  | 2.33                     | 0.59              |
| 11:A40:437:LEU:CD1   | 11:A40:454:LYS:NZ    | 2.66                     | 0.59              |
| 14:W:714:LEU:C       | 10:C8:1568:ARG:NH1   | 2.59                     | 0.59              |
| 10:C:982:LEU:O       | 10:C:990:PHE:CE2     | 2.56                     | 0.59              |
| 11:A16:714:GLY:CA    | 24:D16:1398:ARG:CZ   | 2.80                     | 0.59              |
| 18:B:495:THR:CG2     | 18:B:549:TRP:HE1     | 2.15                     | 0.59              |
| 18:B8:495:THR:CG2    | 18:B8:549:TRP:HE1    | 2.15                     | 0.59              |
| 18:B8:719:GLU:OE2    | 18:B8:766:LYS:CE     | 2.51                     | 0.59              |
| 18:B8:854:SER:O      | 18:B8:855:GLY:O      | 2.21                     | 0.59              |
| 19:4:419:PHE:HE2     | 19:4:424:LEU:HD11    | 1.68                     | 0.59              |
| 22:I24:182:MET:HE1   | 23:J24:605:LEU:HD23  | 1.85                     | 0.59              |
| 21:H16:287:ILE:HG23  | 22:I16:273:LEU:CD1   | 2.31                     | 0.59              |
| 22:I16:182:MET:CE    | 23:J16:605:LEU:HD23  | 2.33                     | 0.59              |
| 10:C32:1807:LEU:HD23 | 10:C32:1810:LEU:HD11 | 1.85                     | 0.59              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R:1139:ARG:CB     | 1:R:1157:ARG:CZ      | 2.81                     | 0.58              |
| 1:R:1204:ASN:C      | 1:R:1206:GLN:H       | 2.11                     | 0.58              |
| 1:R:1266:THR:CA     | 5:P:684:ARG:HH21     | 2.16                     | 0.58              |
| 2:M:757:VAL:HG12    | 2:M:758:GLU:N        | 2.18                     | 0.58              |
| 1:R8:1099:ALA:O     | 1:R8:1137:ARG:NH1    | 2.36                     | 0.58              |
| 5:P:477:GLN:OE1     | 5:P:511:LYS:HE2      | 2.03                     | 0.58              |
| 5:P8:620:ILE:CG2    | 5:P8:660:ARG:NH2     | 2.66                     | 0.58              |
| 5:P16:220:GLU:CD    | 5:P16:232:ARG:HH12   | 2.11                     | 0.58              |
| 5:P16:477:GLN:OE1   | 5:P16:511:LYS:HE2    | 2.03                     | 0.58              |
| 6:O16:23:ARG:HG2    | 6:O16:37:GLU:HG2     | 1.84                     | 0.58              |
| 9:K8:912:TYR:CE2    | 9:K8:961:ILE:HG12    | 2.39                     | 0.58              |
| 9:K16:649:MET:HA    | 9:K16:704:ARG:HH21   | 1.67                     | 0.58              |
| 10:C16:717:GLU:HG2  | 23:J8:656:ARG:NE     | 2.17                     | 0.58              |
| 10:C24:736:ILE:HD11 | 10:C24:794:LYS:HZ2   | 1.68                     | 0.58              |
| 10:C24:1519:ARG:NH2 | 10:C24:1578:LEU:HB2  | 2.18                     | 0.58              |
| 11:A40:590:TYR:CD2  | 11:A40:623:LEU:HB3   | 2.38                     | 0.58              |
| 12:A:302:GLN:HE22   | 12:A:324:ARG:NH1     | 1.96                     | 0.58              |
| 12:A:388:VAL:HG12   | 12:A:392:SER:HB2     | 1.85                     | 0.58              |
| 10:C:653:TYR:N      | 10:C:654:PRO:CD      | 2.66                     | 0.58              |
| 10:C8:16:LEU:CD2    | 10:C8:139:ARG:NH1    | 2.66                     | 0.58              |
| 10:C8:898:GLN:HG3   | 10:C8:1138:GLU:CG    | 2.33                     | 0.58              |
| 11:A32:578:LEU:HD11 | 11:A32:630:ARG:HG3   | 1.85                     | 0.58              |
| 18:B:273:MET:HG3    | 18:B:390:HIS:HD2     | 1.67                     | 0.58              |
| 18:B:719:GLU:OE2    | 18:B:766:LYS:CE      | 2.51                     | 0.58              |
| 18:B8:749:HIS:HA    | 18:B8:752:TRP:CD2    | 2.38                     | 0.58              |
| 18:B8:1438:LEU:HD13 | 18:B8:1462:LEU:HD11  | 1.84                     | 0.58              |
| 20:E:353:ILE:HD12   | 20:E:413:PHE:O       | 2.03                     | 0.58              |
| 19:48:423:PRO:HD2   | 19:48:441:PHE:CE1    | 2.38                     | 0.58              |
| 20:E8:408:LEU:CD1   | 20:E8:507:LEU:HD23   | 2.33                     | 0.58              |
| 20:E8:418:THR:C     | 20:E8:420:LEU:H      | 2.11                     | 0.58              |
| 21:H:287:ILE:HG23   | 22:I:273:LEU:CD1     | 2.32                     | 0.58              |
| 24:D:308:ASN:CG     | 24:D16:753:ARG:NH2   | 2.60                     | 0.58              |
| 10:C32:407:LYS:HG3  | 10:C32:465:PHE:HE1   | 1.64                     | 0.58              |
| 10:C32:962:PHE:HE2  | 10:C32:997:ILE:CD1   | 2.16                     | 0.58              |
| 10:C32:1010:ALA:HA  | 10:C32:1192:ARG:HH21 | 1.65                     | 0.58              |
| 1:R:1324:ASP:OD1    | 10:C:1180:ILE:CG2    | 2.51                     | 0.58              |
| 2:M:202:LYS:CE      | 2:M:206:SER:HG       | 2.11                     | 0.58              |
| 2:M:847:PHE:CB      | 4:T:656:TRP:CE3      | 2.32                     | 0.58              |
| 1:R8:1188:TYR:OH    | 24:D40:1459:LEU:CD1  | 2.48                     | 0.58              |
| 1:R8:1428:VAL:HG13  | 1:R8:1431:ARG:NE     | 2.18                     | 0.58              |
| 1:R16:1099:ALA:O    | 1:R16:1137:ARG:NH1   | 2.37                     | 0.58              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M16:417:ARG:HB2    | 8:L16:298:PHE:HE2    | 1.60                     | 0.58              |
| 5:P:10:GLY:HA2       | 5:P:26:TYR:OH        | 2.02                     | 0.58              |
| 5:P:318:THR:CG2      | 13:V:763:LYS:HZ2     | 2.13                     | 0.58              |
| 5:P8:214:LEU:HD23    | 5:P8:236:VAL:HG13    | 1.81                     | 0.58              |
| 5:P8:247:GLU:OE1     | 5:P8:295:LYS:HA      | 2.03                     | 0.58              |
| 5:P8:477:GLN:OE1     | 5:P8:511:LYS:HE2     | 2.03                     | 0.58              |
| 9:K:999:PHE:CD1      | 9:K:1023:LEU:HD21    | 2.39                     | 0.58              |
| 9:K:1198:LEU:HD11    | 9:K:1267:LEU:CD2     | 2.28                     | 0.58              |
| 10:C16:1708:ARG:HG3  | 10:C16:1730:ILE:CD1  | 2.33                     | 0.58              |
| 11:A24:694:GLU:OE2   | 24:D8:1397:THR:C     | 2.46                     | 0.58              |
| 10:C24:1318:ARG:HD3  | 10:C24:1398:PHE:CD1  | 2.37                     | 0.58              |
| 10:C24:1535:LEU:HB3  | 10:C24:1548:ILE:HD13 | 1.85                     | 0.58              |
| 10:C:8:VAL:HG23      | 10:C:129:ASP:O       | 2.02                     | 0.58              |
| 10:C:1439:ILE:CD1    | 10:C:1457:LEU:CD1    | 2.75                     | 0.58              |
| 10:C8:8:VAL:HG23     | 10:C8:129:ASP:O      | 2.02                     | 0.58              |
| 10:C8:667:ILE:HA     | 10:C8:670:GLU:H      | 1.68                     | 0.58              |
| 10:C8:1050:HIS:CE1   | 10:C8:1086:LYS:HZ1   | 2.18                     | 0.58              |
| 10:C8:1283:LEU:O     | 10:C8:1287:MET:N     | 2.33                     | 0.58              |
| 11:A16:578:LEU:HD11  | 11:A16:630:ARG:HG3   | 1.85                     | 0.58              |
| 11:A32:557:LEU:HD23  | 11:A32:561:ASP:HB3   | 1.85                     | 0.58              |
| 19:4:63:GLY:O        | 19:4:64:ASP:C        | 2.37                     | 0.58              |
| 19:4:244:GLN:NE2     | 20:E:364:PHE:CD1     | 2.70                     | 0.58              |
| 19:48:110:GLY:HA2    | 19:48:418:LYS:HE3    | 1.84                     | 0.58              |
| 22:I:96:PHE:CE2      | 22:I:113:HIS:CG      | 2.91                     | 0.58              |
| 22:I8:182:MET:HE1    | 23:J8:605:LEU:HD23   | 1.85                     | 0.58              |
| 24:D8:472:ILE:HD11   | 24:D8:539:THR:HG22   | 1.85                     | 0.58              |
| 10:C32:1519:ARG:NH2  | 10:C32:1578:LEU:HB2  | 2.18                     | 0.58              |
| 10:C32:1614:LEU:HD11 | 10:C32:1635:LEU:CD2  | 2.32                     | 0.58              |
| 10:C32:1708:ARG:HA   | 10:C32:1730:ILE:HD11 | 1.85                     | 0.58              |
| 1:R:1166:ASN:HD21    | 5:P:672:LEU:HD22     | 1.60                     | 0.58              |
| 2:M:354:ASP:C        | 2:M:356:GLU:N        | 2.60                     | 0.58              |
| 2:M:672:TYR:CG       | 2:M:680:LYS:CE       | 2.86                     | 0.58              |
| 5:P:47:ASN:OD1       | 5:P:471:SER:CB       | 2.50                     | 0.58              |
| 6:O8:119:ARG:HG3     | 6:O8:181:GLU:O       | 2.03                     | 0.58              |
| 9:K:912:TYR:CE2      | 9:K:961:ILE:HG12     | 2.38                     | 0.58              |
| 10:C16:1290:HIS:CD2  | 10:C16:1334:MET:HE3  | 2.26                     | 0.58              |
| 10:C16:1290:HIS:HD2  | 10:C16:1334:MET:HE2  | 1.66                     | 0.58              |
| 10:C16:1547:LYS:CD   | 24:D8:1406:SER:HB2   | 2.32                     | 0.58              |
| 11:A24:437:LEU:CD1   | 11:A24:454:LYS:HZ3   | 2.16                     | 0.58              |
| 10:C24:278:ARG:NH1   | 10:C24:327:ILE:CG2   | 2.67                     | 0.58              |
| 10:C24:847:ARG:NH2   | 10:C24:910:SER:CB    | 2.59                     | 0.58              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1036:SER:HB2 | 10:C24:1040:HIS:HB3  | 1.86                     | 0.58              |
| 10:C24:1274:ALA:C   | 10:C24:1276:SER:N    | 2.48                     | 0.58              |
| 10:C24:1728:ASP:O   | 21:H24:275:LYS:HE3   | 2.03                     | 0.58              |
| 11:A40:156:MET:CA   | 11:A40:555:HIS:NE2   | 2.65                     | 0.58              |
| 12:A:590:TYR:CD2    | 12:A:623:LEU:HB3     | 2.38                     | 0.58              |
| 14:W:265:MET:HE2    | 14:W:301:LEU:CD2     | 2.34                     | 0.58              |
| 10:C:278:ARG:NH1    | 10:C:327:ILE:CG2     | 2.67                     | 0.58              |
| 10:C:919:ASP:H      | 10:C:927:THR:CG2     | 2.16                     | 0.58              |
| 10:C:1111:SER:C     | 10:C:1113:LYS:N      | 2.58                     | 0.58              |
| 10:C:1318:ARG:HD3   | 10:C:1398:PHE:CD1    | 2.37                     | 0.58              |
| 10:C:1614:LEU:HD11  | 10:C:1635:LEU:CD2    | 2.32                     | 0.58              |
| 10:C8:663:ILE:HG22  | 10:C8:667:ILE:CG2    | 2.33                     | 0.58              |
| 10:C8:1708:ARG:HA   | 10:C8:1730:ILE:HD11  | 1.85                     | 0.58              |
| 11:A16:590:TYR:CD2  | 11:A16:623:LEU:HB3   | 2.38                     | 0.58              |
| 11:A16:845:THR:OG1  | 24:D16:1297:HIS:CE1  | 2.56                     | 0.58              |
| 11:A32:288:HIS:HB2  | 11:A32:354:ARG:HH12  | 1.64                     | 0.58              |
| 18:B:749:HIS:HA     | 18:B:752:TRP:CD2     | 2.38                     | 0.58              |
| 18:B:1575:GLN:NE2   | 24:D16:1403:LEU:HG   | 2.17                     | 0.58              |
| 18:B8:1264:GLN:HE22 | 18:B8:1394:TRP:HZ3   | 1.50                     | 0.58              |
| 20:E:350:GLU:HB3    | 20:E:352:PHE:HD2     | 1.67                     | 0.58              |
| 10:C32:582:GLU:HG3  | 10:C32:637:TYR:CE2   | 2.37                     | 0.58              |
| 10:C32:1530:PHE:O   | 10:C32:1533:THR:OG1  | 2.20                     | 0.58              |
| 10:C32:1535:LEU:HB3 | 10:C32:1548:ILE:HD13 | 1.85                     | 0.58              |
| 12:A48:288:HIS:HB2  | 12:A48:354:ARG:HH12  | 1.64                     | 0.58              |
| 12:A48:322:ARG:NH1  | 12:A48:351:PHE:CZ    | 2.72                     | 0.58              |
| 1:R:1428:VAL:HG13   | 1:R:1431:ARG:NE      | 2.18                     | 0.58              |
| 2:M:247:PRO:N       | 2:M:290:ILE:HD13     | 2.19                     | 0.58              |
| 2:M8:377:ARG:HH12   | 2:M8:477:ASP:HB2     | 1.61                     | 0.58              |
| 2:M8:627:TYR:HD1    | 2:M8:627:TYR:N       | 2.00                     | 0.58              |
| 3:N8:263:TRP:NE1    | 3:N8:279:GLY:HA2     | 2.18                     | 0.58              |
| 5:P:109:ILE:CD1     | 14:W:18:PRO:CB       | 2.81                     | 0.58              |
| 7:Q:211:GLY:O       | 7:Q:212:GLU:HG3      | 2.04                     | 0.58              |
| 7:Q8:142:TRP:CD2    | 7:Q8:148:CYS:HB3     | 2.38                     | 0.58              |
| 5:P16:505:GLU:OE1   | 6:O16:41:SER:HB3     | 2.03                     | 0.58              |
| 7:Q16:142:TRP:CD2   | 7:Q16:148:CYS:HB3    | 2.38                     | 0.58              |
| 9:K8:1214:TYR:HB2   | 9:K8:1269:CYS:SG     | 2.42                     | 0.58              |
| 10:C16:278:ARG:NH1  | 10:C16:327:ILE:CG2   | 2.67                     | 0.58              |
| 10:C24:1126:ASP:CG  | 24:D24:1069:GLY:HA3  | 2.28                     | 0.58              |
| 11:A40:322:ARG:NH1  | 11:A40:351:PHE:CZ    | 2.72                     | 0.58              |
| 18:B:854:SER:O      | 18:B:855:GLY:O       | 2.22                     | 0.58              |
| 20:E:433:LYS:C      | 20:E:435:ALA:N       | 2.60                     | 0.58              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 19:48:304:ILE:CD1    | 19:48:359:ALA:HA     | 2.33                     | 0.58              |
| 22:I:96:PHE:HE2      | 22:I:113:HIS:CG      | 2.21                     | 0.58              |
| 22:I:182:MET:CE      | 23:J32:605:LEU:HD23  | 2.33                     | 0.58              |
| 22:I:182:MET:HE1     | 23:J32:605:LEU:HD23  | 1.85                     | 0.58              |
| 21:H24:240:ILE:HD13  | 22:I24:174:GLN:OE1   | 2.02                     | 0.58              |
| 22:I24:96:PHE:HE2    | 22:I24:113:HIS:CG    | 2.21                     | 0.58              |
| 22:I16:207:PRO:C     | 22:I16:209:TRP:N     | 2.60                     | 0.58              |
| 24:D24:472:ILE:HD11  | 24:D24:539:THR:HG22  | 1.85                     | 0.58              |
| 10:C32:663:ILE:HG22  | 10:C32:667:ILE:HG23  | 1.85                     | 0.58              |
| 10:C32:1230:TYR:HB2  | 10:C32:1291:LEU:HD21 | 1.85                     | 0.58              |
| 1:R:1324:ASP:OD2     | 10:C:1180:ILE:CB     | 2.50                     | 0.58              |
| 2:M8:173:SER:OG      | 3:N8:234:GLN:NE2     | 2.31                     | 0.58              |
| 2:M16:377:ARG:NH1    | 2:M16:477:ASP:HB2    | 2.11                     | 0.58              |
| 2:M16:385:LEU:HD11   | 2:M16:396:PHE:HE2    | 1.58                     | 0.58              |
| 2:M16:641:CYS:SG     | 2:M16:668:LEU:HD23   | 2.42                     | 0.58              |
| 3:N16:208:LYS:HB3    | 3:N16:239:ILE:CD1    | 2.34                     | 0.58              |
| 5:P:56:ASN:CB        | 5:P:59:LEU:HD12      | 2.27                     | 0.58              |
| 6:O:119:ARG:HG3      | 6:O:181:GLU:O        | 2.03                     | 0.58              |
| 7:Q:142:TRP:CD2      | 7:Q:148:CYS:HB3      | 2.38                     | 0.58              |
| 5:P8:303:LYS:HB3     | 5:P8:304:PRO:HD3     | 1.84                     | 0.58              |
| 5:P16:620:ILE:HG23   | 5:P16:660:ARG:HH21   | 1.68                     | 0.58              |
| 6:O16:179:LYS:HB3    | 6:O16:183:GLN:HB2    | 1.86                     | 0.58              |
| 8:L16:173:ASP:HB2    | 12:A48:783:PHE:HE1   | 1.66                     | 0.58              |
| 10:C16:743:PHE:CZ    | 10:C16:749:LEU:CD2   | 2.87                     | 0.58              |
| 10:C16:1036:SER:HB2  | 10:C16:1040:HIS:HB3  | 1.85                     | 0.58              |
| 10:C16:1230:TYR:HB2  | 10:C16:1291:LEU:HD21 | 1.85                     | 0.58              |
| 10:C16:1821:VAL:HG11 | 11:A24:144:LYS:HE2   | 1.86                     | 0.58              |
| 11:A24:437:LEU:CD1   | 11:A24:454:LYS:NZ    | 2.66                     | 0.58              |
| 11:A24:696:ILE:CD1   | 11:A24:728:ILE:CD1   | 2.82                     | 0.58              |
| 10:C24:582:GLU:HG3   | 10:C24:637:TYR:CE2   | 2.38                     | 0.58              |
| 10:C24:743:PHE:CZ    | 10:C24:749:LEU:CD2   | 2.87                     | 0.58              |
| 10:C24:1230:TYR:HB2  | 10:C24:1291:LEU:HD21 | 1.85                     | 0.58              |
| 12:A:109:HIS:NE2     | 10:C:1212:GLU:OE1    | 2.26                     | 0.58              |
| 10:C8:420:TYR:CE1    | 10:C8:435:SER:HB3    | 2.39                     | 0.58              |
| 10:C8:1535:LEU:HB3   | 10:C8:1548:ILE:HD13  | 1.85                     | 0.58              |
| 18:B:1529:GLU:OE2    | 24:D16:1415:LEU:HD21 | 2.04                     | 0.58              |
| 18:B8:273:MET:HG3    | 18:B8:390:HIS:HD2    | 1.67                     | 0.58              |
| 18:B8:1668:PHE:CZ    | 18:B8:1731:PHE:HD2   | 2.22                     | 0.58              |
| 21:H16:363:MET:HA    | 21:H16:366:MET:HE3   | 1.85                     | 0.58              |
| 10:C32:653:TYR:N     | 10:C32:654:PRO:CD    | 2.66                     | 0.58              |
| 2:M:816:ARG:HH22     | 2:M:849:LEU:HD22     | 1.68                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M16:554:PHE:CE2   | 2:M16:555:LEU:HG    | 2.39                     | 0.58              |
| 5:P:187:TRP:CZ3     | 5:P:191:ARG:HD3     | 2.38                     | 0.58              |
| 5:P16:538:LYS:HD3   | 6:O16:86:GLU:OE1    | 2.04                     | 0.58              |
| 5:P16:645:LEU:HB3   | 5:P16:646:PRO:HD3   | 1.85                     | 0.58              |
| 8:L8:557:PHE:HB2    | 8:L8:634:HIS:CD2    | 2.38                     | 0.58              |
| 8:L8:1089:MET:CE    | 9:K8:1000:SER:HB2   | 2.24                     | 0.58              |
| 8:L16:1026:ARG:HE   | 9:K16:1284:MET:HE3  | 1.67                     | 0.58              |
| 9:K:635:ALA:CB      | 9:K:655:GLN:CD      | 2.63                     | 0.58              |
| 9:K:703:LEU:CD1     | 9:K:805:ILE:HD11    | 2.33                     | 0.58              |
| 9:K8:703:LEU:CD1    | 9:K8:805:ILE:HD11   | 2.33                     | 0.58              |
| 9:K8:842:ILE:CG2    | 9:K8:871:LEU:HD21   | 2.33                     | 0.58              |
| 10:C16:582:GLU:HG3  | 10:C16:637:TYR:CE2  | 2.38                     | 0.58              |
| 10:C16:1519:ARG:NH2 | 10:C16:1578:LEU:HB2 | 2.18                     | 0.58              |
| 11:A24:246:SER:HB2  | 17:F:61:THR:OG1     | 2.04                     | 0.58              |
| 11:A40:246:SER:HB2  | 17:F16:61:THR:OG1   | 2.04                     | 0.58              |
| 12:A:353:LEU:HD11   | 12:A:381:TRP:CZ3    | 2.39                     | 0.58              |
| 13:V:817:GLN:C      | 13:V:819:ALA:N      | 2.57                     | 0.58              |
| 10:C:1023:LEU:HD22  | 10:C:1210:ILE:CD1   | 2.34                     | 0.58              |
| 10:C8:510:TRP:N     | 10:C8:511:PRO:CD    | 2.66                     | 0.58              |
| 10:C8:960:PHE:CZ    | 10:C8:1138:GLU:CB   | 2.87                     | 0.58              |
| 10:C8:1111:SER:OG   | 10:C8:1114:TYR:CD2  | 2.57                     | 0.58              |
| 10:C8:1318:ARG:HD3  | 10:C8:1398:PHE:CD1  | 2.37                     | 0.58              |
| 11:A32:515:LEU:HB3  | 11:A32:516:PRO:HD3  | 1.84                     | 0.58              |
| 18:B:1668:PHE:CZ    | 18:B:1731:PHE:HD2   | 2.22                     | 0.58              |
| 18:B8:1101:TYR:CD2  | 18:B8:1132:TRP:CZ3  | 2.92                     | 0.58              |
| 19:4:189:LEU:HD22   | 19:4:203:LEU:HD21   | 1.83                     | 0.58              |
| 20:E:429:PRO:HG2    | 24:D:69:VAL:HG22    | 1.85                     | 0.58              |
| 21:H8:363:MET:HA    | 21:H8:366:MET:HE3   | 1.85                     | 0.58              |
| 21:H24:363:MET:HA   | 21:H24:366:MET:HE3  | 1.85                     | 0.58              |
| 24:D:403:ARG:O      | 24:D16:748:GLU:OE1  | 2.21                     | 0.58              |
| 10:C32:743:PHE:CZ   | 10:C32:749:LEU:CD2  | 2.87                     | 0.58              |
| 12:A48:578:LEU:HD11 | 12:A48:630:ARG:HG3  | 1.85                     | 0.58              |
| 1:R:1099:ALA:O      | 1:R:1137:ARG:NH1    | 2.36                     | 0.58              |
| 1:R:1428:VAL:CB     | 6:O:165:LYS:NZ      | 2.67                     | 0.58              |
| 2:M:554:PHE:CE2     | 2:M:555:LEU:HG      | 2.39                     | 0.58              |
| 3:N:256:LYS:HD2     | 3:N:286:TRP:CH2     | 2.39                     | 0.58              |
| 2:M8:217:ILE:CD1    | 3:N8:8:THR:HG21     | 2.33                     | 0.58              |
| 2:M8:377:ARG:NH1    | 2:M8:477:ASP:HB2    | 2.11                     | 0.58              |
| 2:M8:816:ARG:HH22   | 2:M8:849:LEU:HD22   | 1.68                     | 0.58              |
| 5:P:12:GLU:C        | 5:P:14:VAL:N        | 2.60                     | 0.58              |
| 7:Q:341:GLN:CB      | 10:C8:751:ARG:NH1   | 2.65                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:Q8:258:ARG:C      | 7:Q8:259:TRP:HD1    | 2.11                     | 0.58              |
| 6:O16:119:ARG:HG3   | 6:O16:181:GLU:O     | 2.03                     | 0.58              |
| 7:Q16:200:PHE:HA    | 7:Q16:230:VAL:HG23  | 1.85                     | 0.58              |
| 7:Q16:211:GLY:O     | 7:Q16:212:GLU:HG3   | 2.04                     | 0.58              |
| 9:K:792:LEU:HD11    | 9:K:864:ILE:CD1     | 2.05                     | 0.58              |
| 11:A40:493:TYR:OH   | 17:F16:57:PRO:O     | 2.17                     | 0.58              |
| 11:A40:694:GLU:OE2  | 24:D24:1397:THR:C   | 2.47                     | 0.58              |
| 13:V:906:LEU:HA     | 14:W:784:LEU:HD12   | 1.86                     | 0.58              |
| 10:C:453:LEU:HB3    | 10:C:459:LEU:HD22   | 1.85                     | 0.58              |
| 10:C:510:TRP:N      | 10:C:511:PRO:CD     | 2.66                     | 0.58              |
| 10:C:1230:TYR:HB2   | 10:C:1291:LEU:HD21  | 1.85                     | 0.58              |
| 10:C:1616:ILE:C     | 10:C:1618:SER:H     | 2.11                     | 0.58              |
| 10:C8:453:LEU:HB3   | 10:C8:459:LEU:HD22  | 1.85                     | 0.58              |
| 10:C8:743:PHE:CE2   | 10:C8:749:LEU:CD2   | 2.86                     | 0.58              |
| 11:A16:353:LEU:HD11 | 11:A16:381:TRP:CZ3  | 2.39                     | 0.58              |
| 11:A32:302:GLN:HE22 | 11:A32:324:ARG:HH11 | 1.49                     | 0.58              |
| 11:A32:353:LEU:HD11 | 11:A32:381:TRP:CZ3  | 2.39                     | 0.58              |
| 18:B:684:ILE:HD11   | 24:D16:1065:ALA:HB3 | 1.85                     | 0.58              |
| 18:B:1101:TYR:CD2   | 18:B:1132:TRP:CZ3   | 2.92                     | 0.58              |
| 18:B8:282:GLU:HG3   | 18:B8:444:VAL:HG21  | 1.84                     | 0.58              |
| 18:B8:682:TYR:C     | 18:B8:684:ILE:N     | 2.60                     | 0.58              |
| 18:B8:856:LEU:HD11  | 18:B8:907:SER:CB    | 2.32                     | 0.58              |
| 18:B8:1342:LEU:HD23 | 18:B8:1406:ALA:HB3  | 1.82                     | 0.58              |
| 18:B8:1637:VAL:HG21 | 24:D32:1405:GLY:H   | 1.67                     | 0.58              |
| 19:4:178:ASN:OD1    | 20:E:416:LYS:HE2    | 2.03                     | 0.58              |
| 20:E8:353:ILE:HD13  | 20:E8:413:PHE:HD2   | 0.69                     | 0.58              |
| 2:M:211:MET:HE1     | 3:N:280:ASN:HA      | 1.85                     | 0.58              |
| 6:O:179:LYS:HB3     | 6:O:183:GLN:HB2     | 1.86                     | 0.58              |
| 7:Q:258:ARG:C       | 7:Q:259:TRP:HD1     | 2.11                     | 0.58              |
| 5:P8:675:LEU:CD1    | 5:P8:704:LEU:HD12   | 2.34                     | 0.58              |
| 6:O8:179:LYS:HB3    | 6:O8:183:GLN:HB2    | 1.86                     | 0.58              |
| 7:Q8:211:GLY:O      | 7:Q8:212:GLU:HG3    | 2.04                     | 0.58              |
| 6:O16:180:GLY:C     | 6:O16:182:GLU:N     | 2.59                     | 0.58              |
| 8:L16:1031:PRO:HG3  | 8:L16:1068:PHE:HE1  | 1.69                     | 0.58              |
| 9:K:1198:LEU:HD21   | 9:K:1271:GLU:OE1    | 2.03                     | 0.58              |
| 9:K8:751:LEU:CD2    | 9:K8:754:ARG:NH1    | 2.60                     | 0.58              |
| 9:K8:1198:LEU:HD21  | 9:K8:1271:GLU:OE1   | 2.03                     | 0.58              |
| 11:A24:353:LEU:HD11 | 11:A24:381:TRP:CZ3  | 2.39                     | 0.58              |
| 10:C24:1002:LEU:CD1 | 10:C24:1019:ARG:NH1 | 2.64                     | 0.58              |
| 12:A:806:GLN:CG     | 12:A:847:ARG:HH22   | 2.16                     | 0.58              |
| 14:W:714:LEU:O      | 10:C8:1568:ARG:NH2  | 2.36                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:169:GLN:OE1    | 10:C:169:GLN:CA     | 2.44                     | 0.58              |
| 10:C:584:ILE:HG23   | 10:C:588:LEU:HD23   | 1.86                     | 0.58              |
| 10:C:1050:HIS:CE1   | 10:C:1086:LYS:HZ1   | 2.15                     | 0.58              |
| 10:C8:8:VAL:HG23    | 10:C8:133:THR:HG1   | 1.68                     | 0.58              |
| 10:C8:75:GLN:HE21   | 10:C8:112:PRO:CG    | 2.16                     | 0.58              |
| 10:C8:854:LEU:CD2   | 10:C8:911:ILE:HD11  | 2.33                     | 0.58              |
| 11:A16:137:GLU:CG   | 18:B:1901:GLN:NE2   | 2.39                     | 0.58              |
| 11:A16:698:LYS:CD   | 24:D16:1392:MET:O   | 2.51                     | 0.58              |
| 11:A16:713:ASP:CG   | 11:A16:717:ARG:HE   | 2.10                     | 0.58              |
| 11:A32:713:ASP:CG   | 11:A32:717:ARG:HE   | 2.10                     | 0.58              |
| 18:B:682:TYR:C      | 18:B:684:ILE:N      | 2.60                     | 0.58              |
| 18:B:991:ASP:C      | 18:B:993:ALA:N      | 2.62                     | 0.58              |
| 18:B:1227:TYR:CE1   | 18:B:1236:MET:HE1   | 2.38                     | 0.58              |
| 18:B8:195:MET:HE2   | 18:B8:199:LEU:HD23  | 0.59                     | 0.58              |
| 20:E:432:ILE:CG2    | 20:E:434:TRP:CD1    | 2.87                     | 0.58              |
| 20:E8:52:VAL:HG11   | 20:E8:121:VAL:CG2   | 2.33                     | 0.58              |
| 20:E8:352:PHE:HE1   | 20:E8:451:ILE:CD1   | 1.94                     | 0.58              |
| 20:E8:353:ILE:HD12  | 20:E8:413:PHE:O     | 2.03                     | 0.58              |
| 20:E8:432:ILE:CG2   | 20:E8:434:TRP:CD1   | 2.87                     | 0.58              |
| 20:E8:434:TRP:CD1   | 24:D40:72:GLU:CB    | 2.62                     | 0.58              |
| 21:H8:352:LEU:HD21  | 22:I8:318:VAL:HG12  | 1.85                     | 0.58              |
| 22:I24:131:ARG:HE   | 23:J24:557:ARG:HH22 | 1.52                     | 0.58              |
| 2:M8:578:ARG:CZ     | 2:M8:582:GLU:OE2    | 2.50                     | 0.58              |
| 2:M8:757:VAL:HG12   | 2:M8:758:GLU:N      | 2.18                     | 0.58              |
| 7:Q8:309:SER:OG     | 7:Q8:311:ASP:OD1    | 2.20                     | 0.58              |
| 8:L16:1026:ARG:HE   | 9:K16:1284:MET:CE   | 2.16                     | 0.58              |
| 9:K:1232:LEU:CD2    | 9:K:1265:ILE:HG21   | 2.30                     | 0.58              |
| 9:K8:999:PHE:CD1    | 9:K8:1023:LEU:HD21  | 2.39                     | 0.58              |
| 10:C16:561:ASN:OD1  | 10:C16:562:PRO:CD   | 2.50                     | 0.58              |
| 11:A24:388:VAL:HG12 | 11:A24:392:SER:HB2  | 1.85                     | 0.58              |
| 11:A40:388:VAL:HG12 | 11:A40:392:SER:HB2  | 1.85                     | 0.58              |
| 11:A40:578:LEU:HD11 | 11:A40:630:ARG:HG3  | 1.85                     | 0.58              |
| 13:V:783:TRP:HZ2    | 14:W:671:GLU:CG     | 2.16                     | 0.58              |
| 10:C:453:LEU:CD2    | 10:C:459:LEU:CG     | 2.82                     | 0.58              |
| 10:C:966:CYS:CB     | 10:C:1021:TRP:CE3   | 2.86                     | 0.58              |
| 10:C:1111:SER:OG    | 10:C:1114:TYR:CD2   | 2.57                     | 0.58              |
| 10:C8:1336:ALA:C    | 10:C8:1338:ASP:N    | 2.62                     | 0.58              |
| 10:C8:1530:PHE:O    | 10:C8:1533:THR:OG1  | 2.20                     | 0.58              |
| 11:A32:437:LEU:CD1  | 11:A32:454:LYS:NZ   | 2.66                     | 0.58              |
| 18:B:459:PHE:CD2    | 18:B:460:PRO:HA     | 2.39                     | 0.58              |
| 18:B:712:PRO:HG2    | 18:B:759:MET:HE1    | 0.61                     | 0.58              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 18:B:1788:ILE:HG22  | 18:B:1788:ILE:O    | 2.03                     | 0.58              |
| 18:B8:32:LEU:CD2    | 18:B8:36:ILE:HG21  | 2.34                     | 0.58              |
| 20:E8:128:SER:O     | 20:E8:131:PRO:HD2  | 2.04                     | 0.58              |
| 24:D:403:ARG:HB3    | 24:D16:748:GLU:CD  | 2.26                     | 0.58              |
| 10:C32:1336:ALA:C   | 10:C32:1338:ASP:N  | 2.62                     | 0.58              |
| 1:R:768:LEU:HG      | 24:D:1362:VAL:CA   | 2.34                     | 0.58              |
| 2:M:250:LEU:HD13    | 2:M:286:SER:CB     | 2.32                     | 0.58              |
| 2:M:250:LEU:CD1     | 2:M:286:SER:CB     | 2.82                     | 0.58              |
| 2:M:593:HIS:CD2     | 3:N:224:LEU:CD2    | 2.84                     | 0.58              |
| 2:M8:762:LEU:CD1    | 2:M8:813:ASN:HD22  | 2.17                     | 0.58              |
| 3:N8:256:LYS:HD2    | 3:N8:286:TRP:CH2   | 2.39                     | 0.58              |
| 2:M16:757:VAL:HG12  | 2:M16:758:GLU:N    | 2.18                     | 0.58              |
| 5:P:675:LEU:CD1     | 5:P:704:LEU:HD12   | 2.34                     | 0.58              |
| 5:P16:12:GLU:C      | 5:P16:14:VAL:N     | 2.60                     | 0.58              |
| 10:C16:8:VAL:CG2    | 10:C16:133:THR:OG1 | 2.52                     | 0.58              |
| 10:C24:513:LEU:HD13 | 10:C24:549:TYR:CB  | 2.34                     | 0.58              |
| 11:A40:224:PHE:O    | 11:A40:226:PRO:HD3 | 2.04                     | 0.58              |
| 10:C:286:ILE:CG2    | 10:C:292:PHE:CD1   | 2.87                     | 0.58              |
| 10:C:743:PHE:CZ     | 10:C:749:LEU:CD2   | 2.87                     | 0.58              |
| 10:C8:653:TYR:N     | 10:C8:654:PRO:CD   | 2.66                     | 0.58              |
| 18:B:1116:GLU:C     | 18:B:1117:THR:O    | 2.47                     | 0.58              |
| 19:4:103:GLN:OE1    | 19:4:411:LEU:CD1   | 2.51                     | 0.58              |
| 19:48:117:ILE:HG13  | 19:48:150:LEU:HD23 | 1.86                     | 0.58              |
| 22:I8:96:PHE:HE2    | 22:I8:113:HIS:CG   | 2.21                     | 0.58              |
| 22:I8:182:MET:CE    | 23:J8:605:LEU:HD23 | 2.33                     | 0.58              |
| 23:J24:653:LEU:HD23 | 23:J24:656:ARG:NH2 | 2.18                     | 0.58              |
| 24:D:472:ILE:HD11   | 24:D:539:THR:HG22  | 1.85                     | 0.58              |
| 10:C32:8:VAL:CG2    | 10:C32:133:THR:OG1 | 2.52                     | 0.58              |
| 2:M:762:LEU:CD1     | 2:M:813:ASN:HD22   | 2.17                     | 0.57              |
| 1:R8:1188:TYR:CE1   | 24:D40:1459:LEU:CB | 2.86                     | 0.57              |
| 5:P:220:GLU:CD      | 5:P:232:ARG:HH12   | 2.11                     | 0.57              |
| 6:O:224:ASP:OD1     | 6:O:251:LYS:NZ     | 2.36                     | 0.57              |
| 5:P16:96:VAL:CG1    | 5:P16:481:ILE:HD13 | 2.31                     | 0.57              |
| 5:P16:187:TRP:CZ3   | 5:P16:191:ARG:HD3  | 2.38                     | 0.57              |
| 5:P16:261:LEU:HA    | 5:P16:264:LEU:HD12 | 1.86                     | 0.57              |
| 10:C16:390:HIS:CD2  | 10:C16:452:LEU:CD2 | 2.78                     | 0.57              |
| 10:C16:643:LEU:CD2  | 10:C16:675:ASP:CG  | 2.69                     | 0.57              |
| 10:C16:1449:GLU:OE1 | 24:D8:1151:SER:HA  | 2.03                     | 0.57              |
| 10:C24:561:ASN:OD1  | 10:C24:562:PRO:CD  | 2.50                     | 0.57              |
| 10:C24:720:HIS:HE1  | 23:J16:629:ASN:OD1 | 1.87                     | 0.57              |
| 10:C24:1814:LYS:HZ3 | 23:J24:738:MET:CG  | 2.17                     | 0.57              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A:578:LEU:HD11   | 12:A:630:ARG:HG3    | 1.85                     | 0.57              |
| 10:C8:513:LEU:HD13  | 10:C8:549:TYR:CB    | 2.34                     | 0.57              |
| 11:A16:257:GLN:NE2  | 11:A16:263:ASP:CG   | 2.60                     | 0.57              |
| 11:A16:711:ARG:CD   | 24:D16:1398:ARG:HG2 | 2.34                     | 0.57              |
| 11:A32:112:ALA:HB1  | 18:B8:1416:LYS:HZ3  | 1.65                     | 0.57              |
| 11:A32:224:PHE:O    | 11:A32:226:PRO:HD3  | 2.04                     | 0.57              |
| 11:A32:257:GLN:NE2  | 11:A32:263:ASP:CG   | 2.60                     | 0.57              |
| 11:A32:259:ILE:CG2  | 11:A32:276:LEU:CD2  | 2.80                     | 0.57              |
| 11:A32:322:ARG:NH1  | 11:A32:351:PHE:CZ   | 2.72                     | 0.57              |
| 18:B8:728:GLY:O     | 18:B8:1197:VAL:CG2  | 2.52                     | 0.57              |
| 18:B8:1788:ILE:HG22 | 18:B8:1788:ILE:O    | 2.03                     | 0.57              |
| 19:48:322:LEU:HD21  | 19:48:355:ILE:HD13  | 1.86                     | 0.57              |
| 21:H:352:LEU:HD21   | 22:I:318:VAL:HG12   | 1.86                     | 0.57              |
| 22:I:131:ARG:HE     | 23:J32:557:ARG:HH22 | 1.52                     | 0.57              |
| 21:H24:154:VAL:HG13 | 21:H24:188:ARG:CG   | 2.34                     | 0.57              |
| 22:I16:96:PHE:HE2   | 22:I16:113:HIS:CG   | 2.21                     | 0.57              |
| 10:C32:513:LEU:HD13 | 10:C32:549:TYR:CB   | 2.34                     | 0.57              |
| 10:C32:1616:ILE:C   | 10:C32:1618:SER:H   | 2.11                     | 0.57              |
| 2:M8:627:TYR:CG     | 3:N8:167:LEU:HA     | 2.36                     | 0.57              |
| 3:N16:226:LYS:NZ    | 3:N16:288:GLU:OE1   | 2.37                     | 0.57              |
| 3:N16:256:LYS:HD2   | 3:N16:286:TRP:CH2   | 2.39                     | 0.57              |
| 7:Q:200:PHE:HA      | 7:Q:230:VAL:HG23    | 1.86                     | 0.57              |
| 5:P8:259:TYR:OH     | 5:P8:275:GLU:OE2    | 2.22                     | 0.57              |
| 10:C16:420:TYR:CE1  | 10:C16:435:SER:HB3  | 2.39                     | 0.57              |
| 10:C16:584:ILE:HG23 | 10:C16:588:LEU:HD23 | 1.86                     | 0.57              |
| 11:A24:224:PHE:O    | 11:A24:226:PRO:HD3  | 2.04                     | 0.57              |
| 10:C24:719:PRO:C    | 10:C24:721:PHE:N    | 2.62                     | 0.57              |
| 10:C24:1290:HIS:CD2 | 10:C24:1334:MET:HE3 | 2.26                     | 0.57              |
| 10:C24:1336:ALA:C   | 10:C24:1338:ASP:N   | 2.62                     | 0.57              |
| 14:W:586:ILE:CG1    | 15:J:572:ASP:HB2    | 2.34                     | 0.57              |
| 14:W:649:LEU:HD22   | 15:J:575:ILE:CD1    | 2.30                     | 0.57              |
| 10:C:420:TYR:CE1    | 10:C:435:SER:HB3    | 2.38                     | 0.57              |
| 10:C:667:ILE:HA     | 10:C:670:GLU:H      | 1.69                     | 0.57              |
| 10:C:1336:ALA:C     | 10:C:1338:ASP:N     | 2.62                     | 0.57              |
| 10:C:1340:PRO:HG2   | 10:C:1746:GLY:CA    | 2.34                     | 0.57              |
| 10:C:1488:ILE:HD11  | 10:C:1528:LEU:CD2   | 2.34                     | 0.57              |
| 10:C8:584:ILE:HG23  | 10:C8:588:LEU:HD23  | 1.85                     | 0.57              |
| 10:C8:1807:LEU:HD23 | 10:C8:1810:LEU:HD11 | 1.85                     | 0.57              |
| 18:B:1342:LEU:HD23  | 18:B:1406:ALA:HB3   | 1.82                     | 0.57              |
| 18:B8:152:HIS:HB3   | 18:B8:163:ILE:CD1   | 2.28                     | 0.57              |
| 18:B8:478:TRP:HB3   | 18:B8:479:PRO:HD3   | 1.87                     | 0.57              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:990:PRO:O      | 18:B8:992:TRP:N      | 2.37                     | 0.57              |
| 19:4:220:TRP:CE2     | 19:4:227:LEU:HD13    | 2.39                     | 0.57              |
| 19:4:423:PRO:HD2     | 19:4:441:PHE:CE1     | 2.38                     | 0.57              |
| 20:E:347:PRO:C       | 20:E:349:THR:H       | 2.11                     | 0.57              |
| 19:48:103:GLN:OE1    | 19:48:411:LEU:CD1    | 2.51                     | 0.57              |
| 19:48:189:LEU:HD22   | 19:48:203:LEU:HD21   | 1.83                     | 0.57              |
| 21:H:288:THR:OG1     | 23:J32:650:GLN:CG    | 2.52                     | 0.57              |
| 22:I:207:PRO:C       | 22:I:209:TRP:N       | 2.60                     | 0.57              |
| 23:J8:682:ALA:C      | 23:J8:684:ASP:N      | 2.62                     | 0.57              |
| 21:H24:301:ARG:HH21  | 22:I24:284:GLU:CD    | 2.10                     | 0.57              |
| 10:C32:510:TRP:N     | 10:C32:511:PRO:CD    | 2.66                     | 0.57              |
| 12:A48:437:LEU:CD1   | 12:A48:454:LYS:NZ    | 2.66                     | 0.57              |
| 1:R8:1204:ASN:C      | 1:R8:1206:GLN:H      | 2.11                     | 0.57              |
| 2:M16:257:VAL:CG2    | 2:M16:274:VAL:HG21   | 2.34                     | 0.57              |
| 5:P:155:PRO:HA       | 14:W:765:LYS:HE3     | 0.88                     | 0.57              |
| 5:P8:220:GLU:CD      | 5:P8:232:ARG:NH1     | 2.62                     | 0.57              |
| 5:P8:220:GLU:CD      | 5:P8:232:ARG:HH12    | 2.11                     | 0.57              |
| 5:P16:607:PHE:HB3    | 5:P16:629:ARG:HD3    | 1.86                     | 0.57              |
| 5:P16:620:ILE:CG2    | 5:P16:660:ARG:HH21   | 2.18                     | 0.57              |
| 6:O16:224:ASP:OD1    | 6:O16:251:LYS:NZ     | 2.36                     | 0.57              |
| 10:C16:667:ILE:CG1   | 10:C16:670:GLU:H     | 2.17                     | 0.57              |
| 10:C16:1002:LEU:CD2  | 10:C16:1012:ARG:CZ   | 2.79                     | 0.57              |
| 10:C16:1023:LEU:HD22 | 10:C16:1210:ILE:CD1  | 2.34                     | 0.57              |
| 10:C16:1465:LEU:O    | 10:C16:1469:HIS:ND1  | 2.34                     | 0.57              |
| 10:C16:1616:ILE:C    | 10:C16:1618:SER:H    | 2.11                     | 0.57              |
| 10:C16:1708:ARG:NH1  | 21:H:279:GLU:HB2     | 2.18                     | 0.57              |
| 10:C16:1708:ARG:HA   | 10:C16:1730:ILE:HD11 | 1.85                     | 0.57              |
| 11:A24:322:ARG:NH1   | 11:A24:351:PHE:CZ    | 2.72                     | 0.57              |
| 10:C24:8:VAL:CG2     | 10:C24:133:THR:OG1   | 2.52                     | 0.57              |
| 10:C24:420:TYR:CE1   | 10:C24:435:SER:HB3   | 2.39                     | 0.57              |
| 10:C24:653:TYR:N     | 10:C24:654:PRO:CD    | 2.66                     | 0.57              |
| 12:A:322:ARG:NH1     | 12:A:351:PHE:CZ      | 2.72                     | 0.57              |
| 10:C:75:GLN:HE21     | 10:C:112:PRO:CG      | 2.16                     | 0.57              |
| 10:C:1358:ASP:C      | 10:C:1361:LYS:H      | 2.13                     | 0.57              |
| 10:C:1465:LEU:O      | 10:C:1469:HIS:ND1    | 2.34                     | 0.57              |
| 10:C8:278:ARG:NH1    | 10:C8:327:ILE:CG2    | 2.67                     | 0.57              |
| 10:C8:1036:SER:HB2   | 10:C8:1040:HIS:HB3   | 1.85                     | 0.57              |
| 10:C8:1616:ILE:C     | 10:C8:1618:SER:H     | 2.11                     | 0.57              |
| 10:C8:1708:ARG:HG3   | 10:C8:1730:ILE:CD1   | 2.33                     | 0.57              |
| 18:B:782:THR:C       | 24:D16:1066:VAL:HG21 | 2.25                     | 0.57              |
| 18:B:782:THR:C       | 24:D16:1066:VAL:HG23 | 2.29                     | 0.57              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:856:LEU:HD11   | 18:B:907:SER:CB     | 2.32                     | 0.57              |
| 18:B8:459:PHE:CD2   | 18:B8:460:PRO:HA    | 2.39                     | 0.57              |
| 18:B8:750:GLU:CG    | 18:B8:760:ARG:NH2   | 2.67                     | 0.57              |
| 18:B8:1227:TYR:CE1  | 18:B8:1236:MET:HE1  | 2.38                     | 0.57              |
| 23:J32:653:LEU:HD23 | 23:J32:656:ARG:NH2  | 2.18                     | 0.57              |
| 21:H8:194:VAL:HG13  | 21:H8:199:ASP:CB    | 2.34                     | 0.57              |
| 21:H16:352:LEU:HD21 | 22:I16:318:VAL:HG12 | 1.86                     | 0.57              |
| 23:J16:682:ALA:C    | 23:J16:684:ASP:N    | 2.63                     | 0.57              |
| 10:C32:286:ILE:CG2  | 10:C32:292:PHE:CD1  | 2.87                     | 0.57              |
| 10:C32:420:TYR:CE1  | 10:C32:435:SER:HB3  | 2.39                     | 0.57              |
| 10:C32:561:ASN:OD1  | 10:C32:562:PRO:CD   | 2.50                     | 0.57              |
| 10:C32:854:LEU:CD2  | 10:C32:911:ILE:HD11 | 2.33                     | 0.57              |
| 1:R8:1112:LYS:NZ    | 1:R8:1156:GLU:OE1   | 2.29                     | 0.57              |
| 1:R8:1266:THR:OG1   | 5:P8:684:ARG:NH2    | 2.35                     | 0.57              |
| 2:M16:762:LEU:CD1   | 2:M16:813:ASN:HD22  | 2.17                     | 0.57              |
| 5:P:593:GLN:HG2     | 5:P:593:GLN:O       | 2.04                     | 0.57              |
| 5:P8:620:ILE:CG2    | 5:P8:660:ARG:HH21   | 2.18                     | 0.57              |
| 7:Q8:221:TRP:CD1    | 7:Q8:221:TRP:H      | 2.20                     | 0.57              |
| 5:P16:675:LEU:CD1   | 5:P16:704:LEU:HD12  | 2.34                     | 0.57              |
| 9:K:825:GLY:O       | 9:K:889:ARG:NE      | 2.37                     | 0.57              |
| 10:C16:1271:PHE:CZ  | 10:C16:1284:ASP:HB3 | 2.37                     | 0.57              |
| 11:A24:259:ILE:CG2  | 11:A24:276:LEU:CD2  | 2.80                     | 0.57              |
| 11:A24:557:LEU:HD23 | 11:A24:561:ASP:HB3  | 1.85                     | 0.57              |
| 11:A24:578:LEU:HD11 | 11:A24:630:ARG:HG3  | 1.85                     | 0.57              |
| 11:A24:607:ARG:CZ   | 24:D16:914:PHE:CD1  | 2.82                     | 0.57              |
| 10:C24:452:LEU:C    | 10:C24:452:LEU:CD1  | 2.76                     | 0.57              |
| 10:C24:667:ILE:HA   | 10:C24:670:GLU:H    | 1.68                     | 0.57              |
| 11:A40:353:LEU:HD11 | 11:A40:381:TRP:CZ3  | 2.39                     | 0.57              |
| 12:A:257:GLN:NE2    | 12:A:263:ASP:CG     | 2.60                     | 0.57              |
| 13:V:825:GLN:HA     | 14:W:707:LYS:HZ1    | 1.65                     | 0.57              |
| 14:W:714:LEU:C      | 10:C8:1568:ARG:NH2  | 2.62                     | 0.57              |
| 10:C:854:LEU:CD2    | 10:C:911:ILE:HD11   | 2.33                     | 0.57              |
| 10:C:1708:ARG:HG3   | 10:C:1730:ILE:CD1   | 2.33                     | 0.57              |
| 10:C8:1274:ALA:O    | 10:C8:1276:SER:N    | 2.38                     | 0.57              |
| 10:C8:1488:ILE:HD11 | 10:C8:1528:LEU:CD2  | 2.34                     | 0.57              |
| 11:A16:259:ILE:CG2  | 11:A16:276:LEU:CD2  | 2.80                     | 0.57              |
| 11:A32:445:ASN:ND2  | 17:F24:65:ARG:HH12  | 1.99                     | 0.57              |
| 18:B:1058:ILE:HG23  | 18:B:1154:ILE:HD11  | 1.85                     | 0.57              |
| 18:B8:991:ASP:C     | 18:B8:993:ALA:N     | 2.62                     | 0.57              |
| 18:B8:1676:VAL:O    | 18:B8:1677:ARG:C    | 2.44                     | 0.57              |
| 21:H24:288:THR:OG1  | 23:J24:650:GLN:CG   | 2.52                     | 0.57              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:J24:734:PRO:O     | 23:J24:735:LYS:C     | 2.46                     | 0.57              |
| 21:H16:366:MET:HE1   | 22:I16:332:MET:HE2   | 1.83                     | 0.57              |
| 24:D24:857:THR:OG1   | 24:D24:889:LEU:CD1   | 2.52                     | 0.57              |
| 24:D32:472:ILE:HD11  | 24:D32:539:THR:HG22  | 1.86                     | 0.57              |
| 24:D40:472:ILE:HD11  | 24:D40:539:THR:HG22  | 1.85                     | 0.57              |
| 10:C32:453:LEU:CD2   | 10:C32:459:LEU:CG    | 2.82                     | 0.57              |
| 10:C32:864:ALA:HB1   | 10:C32:914:LEU:HD11  | 1.87                     | 0.57              |
| 1:R:1269:LEU:HD11    | 5:P:684:ARG:HD3      | 1.80                     | 0.57              |
| 2:M:349:ASP:O        | 2:M:351:ALA:N        | 2.28                     | 0.57              |
| 2:M16:816:ARG:HH22   | 2:M16:849:LEU:HD22   | 1.68                     | 0.57              |
| 6:O:173:VAL:CG2      | 6:O:189:LEU:HD13     | 2.27                     | 0.57              |
| 5:P16:578:LEU:HD13   | 5:P16:608:LYS:HZ3    | 1.68                     | 0.57              |
| 8:L:1089:MET:SD      | 9:K:1000:SER:HB2     | 2.44                     | 0.57              |
| 9:K:1007:GLU:HG3     | 9:K:1030:PHE:HE1     | 1.70                     | 0.57              |
| 9:K:1207:PHE:HZ      | 9:K:1271:GLU:OE2     | 1.88                     | 0.57              |
| 10:C16:453:LEU:CD2   | 10:C16:459:LEU:CG    | 2.82                     | 0.57              |
| 10:C16:1002:LEU:CD1  | 10:C16:1019:ARG:NH1  | 2.64                     | 0.57              |
| 10:C24:1074:LEU:HD21 | 18:B8:256:VAL:C      | 2.28                     | 0.57              |
| 10:C24:1274:ALA:O    | 10:C24:1276:SER:N    | 2.38                     | 0.57              |
| 10:C24:1337:LEU:HD23 | 11:A40:126:ARG:NH1   | 2.20                     | 0.57              |
| 10:C24:1394:GLN:CD   | 24:D24:1158:SER:CB   | 2.77                     | 0.57              |
| 10:C24:1708:ARG:HA   | 10:C24:1730:ILE:HD11 | 1.85                     | 0.57              |
| 11:A40:386:GLY:O     | 11:A40:459:ARG:CZ    | 2.53                     | 0.57              |
| 12:A:224:PHE:O       | 12:A:226:PRO:HD3     | 2.04                     | 0.57              |
| 12:A:303:ALA:HB2     | 12:A:321:ILE:HD11    | 1.87                     | 0.57              |
| 10:C:325:MET:CE      | 10:C:352:LEU:HD11    | 2.35                     | 0.57              |
| 10:C8:8:VAL:CG2      | 10:C8:133:THR:OG1    | 2.52                     | 0.57              |
| 10:C8:667:ILE:CD1    | 10:C8:697:HIS:CE1    | 2.78                     | 0.57              |
| 10:C8:1230:TYR:HB2   | 10:C8:1291:LEU:HD21  | 1.85                     | 0.57              |
| 11:A16:322:ARG:NH1   | 11:A16:351:PHE:CZ    | 2.72                     | 0.57              |
| 11:A32:246:SER:HB2   | 17:F24:61:THR:OG1    | 2.04                     | 0.57              |
| 11:A32:676:TYR:HE2   | 24:D32:1396:PRO:N    | 2.01                     | 0.57              |
| 18:B:478:TRP:HB3     | 18:B:479:PRO:HD3     | 1.86                     | 0.57              |
| 18:B:728:GLY:O       | 18:B:1197:VAL:CG2    | 2.52                     | 0.57              |
| 18:B:750:GLU:CG      | 18:B:760:ARG:NH2     | 2.67                     | 0.57              |
| 18:B8:463:SER:HB3    | 18:B8:562:ARG:NH1    | 2.19                     | 0.57              |
| 18:B8:536:ILE:HG21   | 18:B8:545:VAL:HG11   | 1.83                     | 0.57              |
| 19:48:63:GLY:O       | 19:48:64:ASP:C       | 2.36                     | 0.57              |
| 19:48:220:TRP:CE2    | 19:48:227:LEU:HD13   | 2.39                     | 0.57              |
| 23:J8:718:GLN:HE22   | 23:J8:737:TRP:HZ3    | 1.43                     | 0.57              |
| 10:C32:643:LEU:CD2   | 10:C32:675:ASP:CG    | 2.69                     | 0.57              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1149:PHE:CE1  | 10:C32:1153:LEU:HD11 | 2.40                     | 0.57              |
| 10:C32:1488:ILE:HD11 | 10:C32:1528:LEU:CD2  | 2.34                     | 0.57              |
| 1:R8:1449:TRP:CE3    | 2:M8:160:LEU:CD1     | 2.81                     | 0.57              |
| 5:P:318:THR:HG22     | 13:V:763:LYS:HZ2     | 1.62                     | 0.57              |
| 5:P:620:ILE:CG2      | 5:P:660:ARG:HH21     | 2.17                     | 0.57              |
| 7:Q:221:TRP:CD1      | 7:Q:221:TRP:H        | 2.20                     | 0.57              |
| 7:Q8:200:PHE:HA      | 7:Q8:230:VAL:HG23    | 1.86                     | 0.57              |
| 5:P16:220:GLU:CD     | 5:P16:232:ARG:NH1    | 2.62                     | 0.57              |
| 8:L:1074:ARG:HD2     | 9:K:1089:LYS:HB2     | 1.86                     | 0.57              |
| 9:K:792:LEU:HG       | 9:K:864:ILE:HD11     | 1.85                     | 0.57              |
| 10:C16:325:MET:CE    | 10:C16:352:LEU:HD11  | 2.35                     | 0.57              |
| 10:C16:513:LEU:HD13  | 10:C16:549:TYR:CB    | 2.34                     | 0.57              |
| 10:C16:1274:ALA:O    | 10:C16:1276:SER:N    | 2.38                     | 0.57              |
| 10:C16:1807:LEU:HD23 | 10:C16:1810:LEU:HD11 | 1.85                     | 0.57              |
| 11:A24:638:LEU:HA    | 11:A24:644:GLY:HA2   | 1.86                     | 0.57              |
| 11:A40:259:ILE:CG2   | 11:A40:276:LEU:CD2   | 2.80                     | 0.57              |
| 11:A40:638:LEU:HA    | 11:A40:644:GLY:HA2   | 1.86                     | 0.57              |
| 15:J:677:GLY:C       | 15:J:678:GLY:O       | 2.46                     | 0.57              |
| 15:J:682:ALA:C       | 15:J:684:ASP:N       | 2.61                     | 0.57              |
| 10:C:513:LEU:HD13    | 10:C:549:TYR:CB      | 2.34                     | 0.57              |
| 10:C:1274:ALA:O      | 10:C:1276:SER:N      | 2.38                     | 0.57              |
| 10:C8:11:VAL:HG21    | 10:C8:133:THR:HG23   | 1.87                     | 0.57              |
| 11:A16:212:LYS:NZ    | 11:A16:585:MET:HE3   | 2.16                     | 0.57              |
| 11:A16:224:PHE:O     | 11:A16:226:PRO:HD3   | 2.04                     | 0.57              |
| 11:A16:246:SER:HB2   | 17:F8:61:THR:OG1     | 2.04                     | 0.57              |
| 11:A16:257:GLN:CD    | 11:A16:263:ASP:OD2   | 2.48                     | 0.57              |
| 17:F8:69:SER:O       | 17:F8:71:GLU:N       | 2.38                     | 0.57              |
| 11:A32:706:SER:HB2   | 24:D32:1398:ARG:CG   | 2.35                     | 0.57              |
| 18:B:32:LEU:CD2      | 18:B:36:ILE:HG21     | 2.34                     | 0.57              |
| 18:B:313:ILE:HD13    | 18:B:331:TRP:CB      | 2.35                     | 0.57              |
| 18:B8:1116:GLU:C     | 18:B8:1117:THR:O     | 2.47                     | 0.57              |
| 20:E8:202:ASP:O      | 20:E8:204:SER:N      | 2.38                     | 0.57              |
| 21:H:284:LEU:O       | 23:J32:650:GLN:NE2   | 2.37                     | 0.57              |
| 21:H8:288:THR:OG1    | 23:J8:650:GLN:CG     | 2.52                     | 0.57              |
| 21:H24:228:LEU:HD11  | 23:J24:593:VAL:CG2   | 2.34                     | 0.57              |
| 21:H16:288:THR:OG1   | 23:J16:650:GLN:CG    | 2.52                     | 0.57              |
| 21:H16:301:ARG:HH21  | 22:I16:284:GLU:CD    | 2.10                     | 0.57              |
| 24:D8:1428:ASN:CG    | 24:D16:968:ILE:HD11  | 2.30                     | 0.57              |
| 24:D16:472:ILE:HD11  | 24:D16:539:THR:HG22  | 1.85                     | 0.57              |
| 10:C32:278:ARG:NH1   | 10:C32:327:ILE:CG2   | 2.67                     | 0.57              |
| 10:C32:1036:SER:HB2  | 10:C32:1040:HIS:HB3  | 1.86                     | 0.57              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1708:ARG:HG3  | 10:C32:1730:ILE:CD1  | 2.33                     | 0.57              |
| 12:A48:386:GLY:O     | 12:A48:459:ARG:CZ    | 2.53                     | 0.57              |
| 1:R:765:ASP:CG       | 24:D:1361:ALA:HB1    | 2.29                     | 0.57              |
| 1:R:1449:TRP:CH2     | 2:M:161:ASP:N        | 2.73                     | 0.57              |
| 2:M:225:ASP:HB2      | 2:M:606:GLN:NE2      | 2.20                     | 0.57              |
| 2:M:420:CYS:CB       | 8:L:391:TRP:CZ3      | 2.87                     | 0.57              |
| 1:R16:634:ARG:NE     | 4:T16:160:HIS:CE1    | 2.72                     | 0.57              |
| 2:M16:339:GLU:OE2    | 4:T8:639:ASP:HA      | 2.04                     | 0.57              |
| 5:P:538:LYS:HD3      | 6:O:86:GLU:OE1       | 2.03                     | 0.57              |
| 6:O8:43:SER:HA       | 7:Q8:45:ASP:CG       | 2.29                     | 0.57              |
| 7:Q8:4:MET:HE2       | 7:Q8:361:PRO:HB2     | 1.87                     | 0.57              |
| 7:Q16:258:ARG:C      | 7:Q16:259:TRP:HD1    | 2.11                     | 0.57              |
| 9:K:955:TYR:CD1      | 9:K:985:PHE:HD2      | 2.22                     | 0.57              |
| 9:K8:614:PHE:C       | 9:K8:683:GLN:HE21    | 2.10                     | 0.57              |
| 9:K8:774:LEU:O       | 9:K8:778:LEU:HB2     | 2.05                     | 0.57              |
| 10:C16:1149:PHE:CE1  | 10:C16:1153:LEU:HD11 | 2.40                     | 0.57              |
| 10:C16:1337:LEU:HD23 | 11:A24:126:ARG:NH1   | 2.20                     | 0.57              |
| 10:C16:1453:ARG:NH2  | 24:D8:1150:GLY:HA2   | 2.02                     | 0.57              |
| 10:C24:62:ILE:CD1    | 10:C24:72:LEU:CD1    | 2.73                     | 0.57              |
| 10:C24:688:TRP:CZ2   | 10:C24:777:LEU:HD13  | 2.40                     | 0.57              |
| 10:C24:1358:ASP:C    | 10:C24:1361:LYS:H    | 2.13                     | 0.57              |
| 11:A40:806:GLN:CG    | 11:A40:847:ARG:HH22  | 2.16                     | 0.57              |
| 12:A:126:ARG:NH1     | 10:C:1337:LEU:HD23   | 2.20                     | 0.57              |
| 12:A:257:GLN:CD      | 12:A:263:ASP:OD2     | 2.48                     | 0.57              |
| 10:C8:169:GLN:O      | 10:C8:173:THR:OG1    | 2.23                     | 0.57              |
| 10:C8:743:PHE:CZ     | 10:C8:749:LEU:CD2    | 2.87                     | 0.57              |
| 10:C8:1821:VAL:HG11  | 16:A8:144:LYS:HE2    | 1.86                     | 0.57              |
| 11:A16:560:MET:HE2   | 11:A16:615:GLN:NE2   | 1.97                     | 0.57              |
| 11:A32:257:GLN:CD    | 11:A32:263:ASP:OD2   | 2.48                     | 0.57              |
| 18:B:1182:LEU:HD13   | 18:B:1202:ILE:HD11   | 1.86                     | 0.57              |
| 21:H8:284:LEU:O      | 23:J8:650:GLN:NE2    | 2.37                     | 0.57              |
| 21:H8:301:ARG:HH21   | 22:I8:284:GLU:CD     | 2.10                     | 0.57              |
| 23:J24:682:ALA:C     | 23:J24:684:ASP:N     | 2.63                     | 0.57              |
| 10:C32:11:VAL:HG21   | 10:C32:133:THR:HG23  | 1.87                     | 0.57              |
| 10:C32:743:PHE:CE2   | 10:C32:749:LEU:HD22  | 2.40                     | 0.57              |
| 10:C32:1023:LEU:HD22 | 10:C32:1210:ILE:CD1  | 2.34                     | 0.57              |
| 10:C32:1821:VAL:HG11 | 12:A48:144:LYS:HE2   | 1.85                     | 0.57              |
| 12:A48:353:LEU:HD11  | 12:A48:381:TRP:CZ3   | 2.39                     | 0.57              |
| 1:R:634:ARG:NE       | 4:T:160:HIS:CE1      | 2.72                     | 0.57              |
| 1:R8:1266:THR:CB     | 5:P8:684:ARG:HH22    | 2.15                     | 0.57              |
| 5:P:261:LEU:HA       | 5:P:264:LEU:HD12     | 1.86                     | 0.57              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 5:P:592:SER:C       | 5:P:594:ILE:N        | 2.56                     | 0.57              |
| 6:O16:163:LEU:C     | 6:O16:164:GLY:O      | 2.48                     | 0.57              |
| 9:K8:825:GLY:O      | 9:K8:889:ARG:NE      | 2.37                     | 0.57              |
| 9:K8:1007:GLU:HG3   | 9:K8:1030:PHE:HE1    | 1.70                     | 0.57              |
| 9:K8:1146:ILE:HD13  | 9:K8:1208:GLN:OE1    | 2.05                     | 0.57              |
| 10:C16:667:ILE:HA   | 10:C16:670:GLU:H     | 1.68                     | 0.57              |
| 10:C16:1111:SER:OG  | 10:C16:1114:TYR:CD2  | 2.57                     | 0.57              |
| 11:A24:468:VAL:HG22 | 24:D16:1103:LEU:CG   | 2.24                     | 0.57              |
| 10:C24:453:LEU:CD2  | 10:C24:459:LEU:CG    | 2.82                     | 0.57              |
| 10:C24:584:ILE:HG23 | 10:C24:588:LEU:HD23  | 1.86                     | 0.57              |
| 10:C24:1111:SER:OG  | 10:C24:1114:TYR:CD2  | 2.57                     | 0.57              |
| 10:C24:1149:PHE:CE1 | 10:C24:1153:LEU:HD11 | 2.40                     | 0.57              |
| 11:A40:257:GLN:NE2  | 11:A40:263:ASP:CG    | 2.60                     | 0.57              |
| 12:A:386:GLY:O      | 12:A:459:ARG:CZ      | 2.53                     | 0.57              |
| 12:A:696:ILE:CD1    | 12:A:728:ILE:CD1     | 2.82                     | 0.57              |
| 14:W:261:TRP:CH2    | 14:W:265:MET:HE3     | 2.39                     | 0.57              |
| 14:W:516:GLN:C      | 14:W:605:ASN:N       | 2.62                     | 0.57              |
| 10:C:847:ARG:CD     | 10:C:903:ASN:OD1     | 2.53                     | 0.57              |
| 10:C:983:SER:HA     | 10:C:990:PHE:HE2     | 1.70                     | 0.57              |
| 10:C:1290:HIS:HD2   | 10:C:1334:MET:HE2    | 1.66                     | 0.57              |
| 10:C:1535:LEU:HB3   | 10:C:1548:ILE:HD13   | 1.85                     | 0.57              |
| 11:A16:557:LEU:HD23 | 11:A16:561:ASP:HB3   | 1.85                     | 0.57              |
| 11:A16:587:VAL:CG2  | 11:A16:636:PHE:HE1   | 2.18                     | 0.57              |
| 11:A32:212:LYS:NZ   | 11:A32:585:MET:HE3   | 2.17                     | 0.57              |
| 11:A32:560:MET:HE2  | 11:A32:615:GLN:NE2   | 1.97                     | 0.57              |
| 11:A32:638:LEU:HA   | 11:A32:644:GLY:HA2   | 1.86                     | 0.57              |
| 18:B:463:SER:HB3    | 18:B:562:ARG:NH1     | 2.19                     | 0.57              |
| 18:B:495:THR:HG22   | 18:B:549:TRP:CD1     | 2.40                     | 0.57              |
| 18:B:1799:VAL:C     | 18:B:1801:GLY:H      | 2.13                     | 0.57              |
| 18:B8:313:ILE:HD13  | 18:B8:331:TRP:CB     | 2.35                     | 0.57              |
| 18:B8:457:SER:HA    | 18:B8:548:ARG:HH12   | 1.59                     | 0.57              |
| 20:E8:297:TRP:CE2   | 20:E8:298:ARG:HG3    | 2.40                     | 0.57              |
| 22:I8:196:VAL:CA    | 23:J8:620:MET:CE     | 2.46                     | 0.57              |
| 21:H24:284:LEU:O    | 23:J24:650:GLN:NE2   | 2.37                     | 0.57              |
| 21:H24:352:LEU:HD21 | 22:I24:318:VAL:HG12  | 1.85                     | 0.57              |
| 21:H16:284:LEU:O    | 23:J16:650:GLN:NE2   | 2.38                     | 0.57              |
| 24:D32:764:GLU:OE1  | 24:D40:620:GLN:OE1   | 2.23                     | 0.57              |
| 24:D40:839:GLU:CB   | 24:D40:971:HIS:ND1   | 2.55                     | 0.57              |
| 10:C32:417:LEU:CB   | 10:C32:472:ASN:HD22  | 2.12                     | 0.57              |
| 10:C32:688:TRP:CZ2  | 10:C32:777:LEU:HD13  | 2.40                     | 0.57              |
| 12:A48:696:ILE:CD1  | 12:A48:728:ILE:CD1   | 2.82                     | 0.57              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:R:1166:ASN:CG     | 5:P:672:LEU:HD22    | 2.30                     | 0.57              |
| 1:R8:1145:LYS:HD2   | 1:R8:1149:HIS:CE1   | 2.40                     | 0.57              |
| 1:R8:1191:LYS:HB3   | 24:D40:1453:GLU:OE1 | 2.05                     | 0.57              |
| 3:N8:226:LYS:NZ     | 3:N8:288:GLU:OE1    | 2.37                     | 0.57              |
| 1:R16:1204:ASN:C    | 1:R16:1206:GLN:H    | 2.11                     | 0.57              |
| 5:P:377:LEU:HD12    | 14:W:23:PRO:HB2     | 1.85                     | 0.57              |
| 5:P:578:LEU:HD13    | 5:P:608:LYS:HZ3     | 1.70                     | 0.57              |
| 5:P:600:PHE:CD2     | 5:P:638:SER:HB3     | 2.28                     | 0.57              |
| 7:Q:266:LEU:HD21    | 7:Q:302:ILE:HD12    | 1.87                     | 0.57              |
| 5:P8:505:GLU:OE1    | 6:O8:41:SER:HB3     | 2.03                     | 0.57              |
| 9:K:1019:ARG:CZ     | 9:K:1059:ARG:HG2    | 2.35                     | 0.57              |
| 9:K8:1206:LEU:HD22  | 9:K8:1265:ILE:HD11  | 1.87                     | 0.57              |
| 10:C16:847:ARG:CD   | 10:C16:903:ASN:OD1  | 2.53                     | 0.57              |
| 10:C16:1336:ALA:C   | 10:C16:1338:ASP:N   | 2.62                     | 0.57              |
| 11:A24:707:LEU:CD1  | 11:A24:767:ARG:HH22 | 2.17                     | 0.57              |
| 10:C24:1002:LEU:CD2 | 10:C24:1012:ARG:CZ  | 2.79                     | 0.57              |
| 10:C8:1023:LEU:HD22 | 10:C8:1210:ILE:CD1  | 2.34                     | 0.57              |
| 10:C8:1149:PHE:CE1  | 10:C8:1153:LEU:HD11 | 2.40                     | 0.57              |
| 10:C8:1465:LEU:O    | 10:C8:1469:HIS:ND1  | 2.34                     | 0.57              |
| 10:C8:1708:ARG:HE   | 10:C8:1733:ARG:NH1  | 2.03                     | 0.57              |
| 11:A16:845:THR:CB   | 24:D16:1297:HIS:HE1 | 2.18                     | 0.57              |
| 11:A32:121:GLN:HE22 | 18:B8:1559:ALA:HB2  | 1.61                     | 0.57              |
| 19:4:117:ILE:HG13   | 19:4:150:LEU:HD23   | 1.86                     | 0.57              |
| 10:C32:847:ARG:CD   | 10:C32:903:ASN:OD1  | 2.53                     | 0.57              |
| 12:A48:303:ALA:HB2  | 12:A48:321:ILE:HD11 | 1.87                     | 0.57              |
| 1:R8:1059:ILE:CG2   | 24:D40:1435:ARG:NH1 | 2.67                     | 0.57              |
| 1:R8:1225:PHE:CE1   | 1:R8:1247:PRO:HB3   | 2.40                     | 0.57              |
| 2:M8:211:MET:HE1    | 3:N8:280:ASN:HA     | 1.85                     | 0.57              |
| 2:M16:408:GLU:HG2   | 8:L16:484:PRO:HG3   | 1.86                     | 0.57              |
| 5:P:505:GLU:OE1     | 6:O:41:SER:HB3      | 2.03                     | 0.57              |
| 6:O:163:LEU:C       | 6:O:164:GLY:O       | 2.48                     | 0.57              |
| 5:P8:261:LEU:HA     | 5:P8:264:LEU:HD12   | 1.86                     | 0.57              |
| 5:P8:675:LEU:CD1    | 5:P8:704:LEU:CD1    | 2.83                     | 0.57              |
| 6:O16:43:SER:HA     | 7:Q16:45:ASP:CG     | 2.29                     | 0.57              |
| 7:Q16:4:MET:HE2     | 7:Q16:361:PRO:HB2   | 1.87                     | 0.57              |
| 8:L8:1041:SER:HB2   | 8:L8:1054:HIS:CE1   | 2.34                     | 0.57              |
| 8:L8:1092:LEU:HD22  | 9:K8:999:PHE:CE2    | 2.40                     | 0.57              |
| 10:C16:743:PHE:CE2  | 10:C16:749:LEU:HD22 | 2.40                     | 0.57              |
| 10:C16:1665:THR:CG2 | 10:C24:1601:TYR:C   | 2.77                     | 0.57              |
| 11:A24:36:ASN:HD22  | 22:I8:293:LYS:HZ3   | 1.50                     | 0.57              |
| 11:A24:257:GLN:NE2  | 11:A24:263:ASP:CG   | 2.60                     | 0.57              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A24:302:GLN:HE22  | 11:A24:324:ARG:HH11 | 1.49                     | 0.57              |
| 11:A24:691:ALA:CA    | 24:D8:1397:THR:HG21 | 2.34                     | 0.57              |
| 10:C24:278:ARG:NH1   | 10:C24:287:SER:CB   | 2.62                     | 0.57              |
| 10:C24:286:ILE:CG2   | 10:C24:292:PHE:CD1  | 2.87                     | 0.57              |
| 10:C24:667:ILE:CG2   | 10:C24:669:GLY:C    | 2.68                     | 0.57              |
| 10:C24:743:PHE:CE2   | 10:C24:749:LEU:HD22 | 2.40                     | 0.57              |
| 10:C24:1449:GLU:OE1  | 24:D24:1151:SER:HB2 | 2.05                     | 0.57              |
| 10:C24:1821:VAL:HG11 | 11:A40:144:LYS:HE2  | 1.86                     | 0.57              |
| 12:A:259:ILE:CG2     | 12:A:276:LEU:CD2    | 2.80                     | 0.57              |
| 12:A:638:LEU:HA      | 12:A:644:GLY:HA2    | 1.86                     | 0.57              |
| 14:W:514:THR:CA      | 14:W:607:ARG:NH1    | 2.68                     | 0.57              |
| 10:C:278:ARG:NH1     | 10:C:287:SER:CB     | 2.62                     | 0.57              |
| 10:C:719:PRO:C       | 10:C:721:PHE:N      | 2.62                     | 0.57              |
| 10:C8:244:ASN:HD22   | 10:C8:263:LEU:CD1   | 2.18                     | 0.57              |
| 10:C8:688:TRP:CZ2    | 10:C8:777:LEU:HD13  | 2.40                     | 0.57              |
| 10:C8:1111:SER:C     | 10:C8:1113:LYS:N    | 2.58                     | 0.57              |
| 11:A32:493:TYR:OH    | 17:F24:57:PRO:O     | 2.17                     | 0.57              |
| 17:F24:69:SER:O      | 17:F24:71:GLU:N     | 2.38                     | 0.57              |
| 18:B:664:LEU:HD11    | 18:B:729:LEU:CD2    | 2.28                     | 0.57              |
| 18:B:990:PRO:O       | 18:B:992:TRP:N      | 2.37                     | 0.57              |
| 18:B:1438:LEU:HD13   | 18:B:1462:LEU:HD11  | 1.85                     | 0.57              |
| 18:B8:1182:LEU:HD13  | 18:B8:1202:ILE:HD11 | 1.87                     | 0.57              |
| 18:B8:1733:SER:HB2   | 18:B8:1868:LEU:HD12 | 1.86                     | 0.57              |
| 18:B8:1806:HIS:C     | 18:B8:1808:GLY:N    | 2.62                     | 0.57              |
| 20:E:350:GLU:HB3     | 20:E:352:PHE:CD2    | 2.40                     | 0.57              |
| 19:48:179:MET:O      | 20:E8:416:LYS:HE3   | 2.05                     | 0.57              |
| 23:J32:682:ALA:C     | 23:J32:684:ASP:N    | 2.63                     | 0.57              |
| 21:H24:194:VAL:HG13  | 21:H24:199:ASP:CB   | 2.35                     | 0.57              |
| 22:I16:196:VAL:CA    | 23:J16:620:MET:CE   | 2.46                     | 0.57              |
| 23:J16:718:GLN:CD    | 23:J16:737:TRP:CH2  | 2.83                     | 0.57              |
| 10:C32:584:ILE:HG23  | 10:C32:588:LEU:HD23 | 1.86                     | 0.57              |
| 10:C32:719:PRO:C     | 10:C32:721:PHE:N    | 2.63                     | 0.57              |
| 12:A48:257:GLN:CD    | 12:A48:263:ASP:OD2  | 2.47                     | 0.57              |
| 2:M8:211:MET:CE      | 3:N8:280:ASN:HA     | 2.35                     | 0.56              |
| 2:M8:554:PHE:CE2     | 2:M8:555:LEU:HG     | 2.39                     | 0.56              |
| 5:P:566:PHE:HZ       | 5:P:597:GLY:C       | 2.13                     | 0.56              |
| 5:P8:538:LYS:HD3     | 6:O8:86:GLU:OE1     | 2.03                     | 0.56              |
| 11:A24:257:GLN:CD    | 11:A24:263:ASP:OD2  | 2.47                     | 0.56              |
| 10:C24:389:LEU:HD23  | 10:C24:447:PHE:CE1  | 2.35                     | 0.56              |
| 10:C24:853:GLY:C     | 10:C24:856:PRO:HD2  | 2.30                     | 0.56              |
| 10:C24:1271:PHE:HE2  | 10:C24:1284:ASP:CA  | 2.18                     | 0.56              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C24:1439:ILE:CD1  | 10:C24:1457:LEU:CD1 | 2.75                     | 0.56              |
| 11:A40:257:GLN:CD    | 11:A40:263:ASP:OD2  | 2.48                     | 0.56              |
| 11:A40:474:LEU:CD1   | 24:D32:1099:ARG:NH1 | 2.48                     | 0.56              |
| 11:A40:587:VAL:CG2   | 11:A40:636:PHE:HE1  | 2.18                     | 0.56              |
| 13:V:836:LEU:HG      | 15:J:648:TYR:CE2    | 2.39                     | 0.56              |
| 10:C:1036:SER:HB2    | 10:C:1040:HIS:HB3   | 1.85                     | 0.56              |
| 10:C:1389:ILE:O      | 10:C:1393:SER:OG    | 2.23                     | 0.56              |
| 10:C8:286:ILE:CG2    | 10:C8:292:PHE:CD1   | 2.87                     | 0.56              |
| 10:C8:1340:PRO:CG    | 10:C8:1746:GLY:HA3  | 2.35                     | 0.56              |
| 17:F16:69:SER:O      | 17:F16:71:GLU:N     | 2.38                     | 0.56              |
| 18:B8:457:SER:CA     | 18:B8:548:ARG:HH11  | 2.15                     | 0.56              |
| 19:4:322:LEU:HD21    | 19:4:355:ILE:HD13   | 1.86                     | 0.56              |
| 19:48:423:PRO:HD2    | 19:48:441:PHE:HE1   | 1.69                     | 0.56              |
| 20:E8:432:ILE:HG22   | 20:E8:434:TRP:CD1   | 2.40                     | 0.56              |
| 23:J8:718:GLN:CD     | 23:J8:737:TRP:CH2   | 2.83                     | 0.56              |
| 22:I24:207:PRO:C     | 22:I24:209:TRP:N    | 2.60                     | 0.56              |
| 10:C32:62:ILE:CD1    | 10:C32:72:LEU:CD1   | 2.73                     | 0.56              |
| 10:C32:667:ILE:HA    | 10:C32:670:GLU:H    | 1.68                     | 0.56              |
| 3:N:256:LYS:HD2      | 3:N:286:TRP:HH2     | 1.70                     | 0.56              |
| 1:R8:634:ARG:NE      | 4:T8:160:HIS:CE1    | 2.72                     | 0.56              |
| 2:M8:225:ASP:HB2     | 2:M8:606:GLN:NE2    | 2.20                     | 0.56              |
| 2:M8:544:LEU:CG      | 2:M8:586:ALA:HB1    | 2.35                     | 0.56              |
| 2:M16:211:MET:CE     | 3:N16:280:ASN:HA    | 2.35                     | 0.56              |
| 2:M16:851:LEU:HD21   | 4:T16:653:GLN:CG    | 2.22                     | 0.56              |
| 6:O:43:SER:HA        | 7:Q:45:ASP:CG       | 2.29                     | 0.56              |
| 5:P8:614:VAL:CB      | 5:P8:629:ARG:NE     | 2.52                     | 0.56              |
| 7:Q8:254:ALA:HB2     | 7:Q8:302:ILE:HD13   | 1.87                     | 0.56              |
| 9:K:792:LEU:HD21     | 9:K:849:LEU:HD22    | 1.87                     | 0.56              |
| 9:K8:987:TYR:CE2     | 9:K8:1016:PHE:HD2   | 2.23                     | 0.56              |
| 10:C16:853:GLY:C     | 10:C16:856:PRO:HD2  | 2.30                     | 0.56              |
| 10:C16:864:ALA:HB1   | 10:C16:914:LEU:HD11 | 1.87                     | 0.56              |
| 10:C16:1271:PHE:HE2  | 10:C16:1284:ASP:CA  | 2.19                     | 0.56              |
| 10:C24:452:LEU:O     | 10:C24:452:LEU:CD1  | 2.42                     | 0.56              |
| 10:C24:847:ARG:CD    | 10:C24:903:ASN:OD1  | 2.53                     | 0.56              |
| 10:C24:1023:LEU:HD22 | 10:C24:1210:ILE:CD1 | 2.34                     | 0.56              |
| 10:C24:1358:ASP:C    | 10:C24:1360:GLN:H   | 2.13                     | 0.56              |
| 10:C24:1488:ILE:HD11 | 10:C24:1528:LEU:CD2 | 2.34                     | 0.56              |
| 10:C24:1548:ILE:CD1  | 24:D24:1407:PHE:HE2 | 1.77                     | 0.56              |
| 10:C24:1708:ARG:HE   | 10:C24:1733:ARG:NH1 | 2.03                     | 0.56              |
| 14:W:586:ILE:HD12    | 15:J:569:ALA:C      | 2.30                     | 0.56              |
| 10:C:1333:HIS:CE1    | 10:C:1337:LEU:HD23  | 2.38                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C8:229:PRO:HG2   | 10:C8:270:THR:HG23  | 1.87                     | 0.56              |
| 10:C8:1796:LEU:HG   | 10:C8:1800:LEU:HD12 | 1.87                     | 0.56              |
| 11:A32:90:PHE:CD2   | 18:B8:1788:ILE:HG12 | 2.40                     | 0.56              |
| 18:B:1806:HIS:C     | 18:B:1808:GLY:N     | 2.62                     | 0.56              |
| 19:48:50:THR:O      | 19:48:52:SER:N      | 2.38                     | 0.56              |
| 20:E8:50:PHE:CZ     | 20:E8:54:HIS:CD2    | 2.93                     | 0.56              |
| 20:E8:407:LEU:CD1   | 20:E8:462:THR:HG23  | 2.35                     | 0.56              |
| 21:H8:154:VAL:HG13  | 21:H8:188:ARG:CG    | 2.35                     | 0.56              |
| 10:C32:1708:ARG:HE  | 10:C32:1733:ARG:NH1 | 2.03                     | 0.56              |
| 12:A48:259:ILE:HG22 | 12:A48:276:LEU:CD2  | 2.36                     | 0.56              |
| 1:R:1124:TRP:HZ2    | 4:T:669:PRO:CG      | 2.13                     | 0.56              |
| 1:R:1185:THR:CG2    | 24:D:1462:PHE:CE2   | 2.87                     | 0.56              |
| 1:R:1269:LEU:CD1    | 5:P:684:ARG:NE      | 2.55                     | 0.56              |
| 1:R:1431:ARG:O      | 2:M:177:VAL:CG1     | 2.54                     | 0.56              |
| 2:M:188:ARG:HB2     | 3:N:264:ARG:NH1     | 2.20                     | 0.56              |
| 2:M:202:LYS:HE2     | 2:M:206:SER:O       | 2.06                     | 0.56              |
| 2:M:820:LEU:C       | 2:M:820:LEU:CD1     | 2.78                     | 0.56              |
| 2:M:844:VAL:HG13    | 4:T:660:LEU:HD11    | 1.88                     | 0.56              |
| 3:N:226:LYS:NZ      | 3:N:288:GLU:OE1     | 2.37                     | 0.56              |
| 1:R8:1165:MET:HE1   | 5:P8:676:GLN:HE21   | 1.70                     | 0.56              |
| 2:M8:534:HIS:NE2    | 2:M8:557:THR:CG2    | 2.68                     | 0.56              |
| 2:M8:628:LEU:HD12   | 3:N8:223:GLY:CA     | 2.19                     | 0.56              |
| 2:M8:851:LEU:HD21   | 4:T8:653:GLN:CG     | 2.22                     | 0.56              |
| 3:N8:256:LYS:HD2    | 3:N8:286:TRP:HH2    | 1.70                     | 0.56              |
| 1:R16:1145:LYS:HD2  | 1:R16:1149:HIS:CE1  | 2.40                     | 0.56              |
| 2:M16:217:ILE:HD11  | 3:N16:8:THR:HG21    | 1.87                     | 0.56              |
| 2:M16:820:LEU:C     | 2:M16:820:LEU:CD1   | 2.78                     | 0.56              |
| 5:P:55:ARG:NH1      | 5:P:64:ASP:HB3      | 2.14                     | 0.56              |
| 7:Q:221:TRP:CH2     | 7:Q:222:PHE:HE2     | 2.24                     | 0.56              |
| 6:O8:61:LYS:NZ      | 6:O8:112:ASP:CG     | 2.48                     | 0.56              |
| 6:O8:163:LEU:C      | 6:O8:164:GLY:O      | 2.48                     | 0.56              |
| 5:P16:566:PHE:HZ    | 5:P16:597:GLY:C     | 2.13                     | 0.56              |
| 5:P16:644:TRP:HB2   | 5:P16:678:LEU:HD11  | 1.87                     | 0.56              |
| 5:P16:675:LEU:CD1   | 5:P16:704:LEU:CD1   | 2.83                     | 0.56              |
| 8:L8:1096:GLU:CG    | 9:K8:996:MET:O      | 2.53                     | 0.56              |
| 9:K8:806:LEU:HD12   | 9:K8:874:VAL:HG11   | 1.88                     | 0.56              |
| 9:K8:923:ILE:HG22   | 9:K8:929:ARG:HH21   | 1.70                     | 0.56              |
| 9:K16:894:LYS:NZ    | 9:K16:1058:GLU:HG3  | 2.20                     | 0.56              |
| 10:C16:278:ARG:NH1  | 10:C16:287:SER:CB   | 2.62                     | 0.56              |
| 10:C16:1234:ASP:CG  | 10:C16:1302:LYS:HZ2 | 2.09                     | 0.56              |
| 10:C16:1234:ASP:OD1 | 10:C16:1302:LYS:NZ  | 2.25                     | 0.56              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1340:PRO:HG2  | 10:C16:1746:GLY:CA   | 2.34                     | 0.56              |
| 10:C16:1488:ILE:HD11 | 10:C16:1528:LEU:CD2  | 2.34                     | 0.56              |
| 11:A24:386:GLY:O     | 11:A24:459:ARG:CZ    | 2.53                     | 0.56              |
| 11:A24:806:GLN:CG    | 11:A24:847:ARG:HH22  | 2.16                     | 0.56              |
| 10:C24:1278:ASP:OD1  | 21:H24:282:GLU:HG2   | 2.05                     | 0.56              |
| 10:C24:1807:LEU:HD23 | 10:C24:1810:LEU:HD11 | 1.85                     | 0.56              |
| 11:A40:303:ALA:HB2   | 11:A40:321:ILE:HD11  | 1.87                     | 0.56              |
| 12:A:643:SER:N       | 12:A:685:ARG:NH1     | 2.53                     | 0.56              |
| 13:V:818:THR:HG23    | 13:V:824:TRP:HE1     | 1.70                     | 0.56              |
| 10:C:244:ASN:HD22    | 10:C:263:LEU:CD1     | 2.18                     | 0.56              |
| 10:C:667:ILE:CG1     | 10:C:670:GLU:H       | 2.17                     | 0.56              |
| 10:C:1002:LEU:CD2    | 10:C:1012:ARG:CZ     | 2.79                     | 0.56              |
| 10:C:1149:PHE:CE1    | 10:C:1153:LEU:HD11   | 2.40                     | 0.56              |
| 10:C8:325:MET:CE     | 10:C8:352:LEU:HD11   | 2.35                     | 0.56              |
| 10:C8:1358:ASP:C     | 10:C8:1361:LYS:H     | 2.13                     | 0.56              |
| 11:A16:845:THR:CB    | 24:D16:1297:HIS:CE1  | 2.89                     | 0.56              |
| 11:A32:702:GLU:OE2   | 24:D32:1395:SER:OG   | 2.19                     | 0.56              |
| 18:B:1390:LEU:HD11   | 18:B:1404:LEU:CD1    | 2.36                     | 0.56              |
| 18:B:1676:VAL:O      | 18:B:1677:ARG:C      | 2.44                     | 0.56              |
| 18:B:1911:LEU:HA     | 18:B:1960:LEU:HD11   | 1.86                     | 0.56              |
| 18:B8:495:THR:HG22   | 18:B8:549:TRP:CD1    | 2.40                     | 0.56              |
| 18:B8:1911:LEU:HA    | 18:B8:1960:LEU:HD11  | 1.87                     | 0.56              |
| 20:E:128:SER:O       | 20:E:131:PRO:HD2     | 2.04                     | 0.56              |
| 20:E:202:ASP:O       | 20:E:204:SER:N       | 2.38                     | 0.56              |
| 20:E:297:TRP:CE2     | 20:E:298:ARG:HG3     | 2.40                     | 0.56              |
| 20:E8:333:ASP:O      | 20:E8:337:THR:OG1    | 2.21                     | 0.56              |
| 21:H8:294:PRO:O      | 21:H8:300:ARG:NH2    | 2.38                     | 0.56              |
| 24:D:400:VAL:HG21    | 24:D16:751:MET:HB2   | 1.87                     | 0.56              |
| 10:C32:229:PRO:HG2   | 10:C32:270:THR:HG23  | 1.87                     | 0.56              |
| 10:C32:244:ASN:HD22  | 10:C32:263:LEU:CD1   | 2.18                     | 0.56              |
| 10:C32:325:MET:CE    | 10:C32:352:LEU:HD11  | 2.35                     | 0.56              |
| 10:C32:667:ILE:HD12  | 10:C32:667:ILE:C     | 2.31                     | 0.56              |
| 10:C32:1271:PHE:HE2  | 10:C32:1284:ASP:HB3  | 1.52                     | 0.56              |
| 10:C32:1274:ALA:O    | 10:C32:1276:SER:N    | 2.38                     | 0.56              |
| 10:C32:1337:LEU:HD23 | 12:A48:126:ARG:NH1   | 2.20                     | 0.56              |
| 10:C32:1541:PHE:CE1  | 10:C32:1649:LYS:CD   | 2.89                     | 0.56              |
| 12:A48:587:VAL:CG2   | 12:A48:636:PHE:HE1   | 2.18                     | 0.56              |
| 2:M8:257:VAL:CG2     | 2:M8:274:VAL:HG21    | 2.34                     | 0.56              |
| 2:M16:537:ILE:HG13   | 2:M16:558:MET:CE     | 2.22                     | 0.56              |
| 5:P8:644:TRP:HB2     | 5:P8:678:LEU:HD11    | 1.87                     | 0.56              |
| 6:O8:224:ASP:OD1     | 6:O8:251:LYS:NZ      | 2.36                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:Q8:219:GLY:O      | 7:Q8:221:TRP:N      | 2.38                     | 0.56              |
| 5:P16:291:LEU:CD1   | 5:P16:299:CYS:SG    | 2.94                     | 0.56              |
| 9:K:1206:LEU:HD22   | 9:K:1265:ILE:HD11   | 1.87                     | 0.56              |
| 10:C16:565:ARG:HA   | 10:C16:568:TRP:CD2  | 2.41                     | 0.56              |
| 10:C16:1285:VAL:HA  | 10:C16:1735:TYR:CE2 | 2.32                     | 0.56              |
| 10:C16:1358:ASP:C   | 10:C16:1360:GLN:H   | 2.14                     | 0.56              |
| 11:A24:11:THR:CG2   | 22:I8:162:GLN:NE2   | 2.67                     | 0.56              |
| 10:C24:864:ALA:HB1  | 10:C24:914:LEU:HD11 | 1.87                     | 0.56              |
| 10:C24:1389:ILE:O   | 10:C24:1393:SER:OG  | 2.23                     | 0.56              |
| 11:A40:607:ARG:NH1  | 24:D32:914:PHE:CE1  | 2.73                     | 0.56              |
| 15:J:683:ILE:C      | 15:J:685:GLY:N      | 2.63                     | 0.56              |
| 10:C:229:PRO:HG2    | 10:C:270:THR:HG23   | 1.87                     | 0.56              |
| 10:C:1246:SER:C     | 10:C:1309:ARG:HH22  | 2.14                     | 0.56              |
| 10:C:1614:LEU:CD1   | 10:C:1635:LEU:HD23  | 2.36                     | 0.56              |
| 10:C8:1246:SER:C    | 10:C8:1309:ARG:HH22 | 2.14                     | 0.56              |
| 10:C8:1389:ILE:O    | 10:C8:1393:SER:OG   | 2.23                     | 0.56              |
| 11:A16:259:ILE:HG22 | 11:A16:276:LEU:CD2  | 2.35                     | 0.56              |
| 11:A32:587:VAL:CG2  | 11:A32:636:PHE:HE1  | 2.18                     | 0.56              |
| 18:B:152:HIS:HB3    | 18:B:163:ILE:CD1    | 2.28                     | 0.56              |
| 18:B:986:ALA:C      | 18:B:988:SER:H      | 2.14                     | 0.56              |
| 18:B:1234:MET:HB2   | 18:B:1235:PRO:HD3   | 1.88                     | 0.56              |
| 18:B:1733:SER:HB2   | 18:B:1868:LEU:HD12  | 1.86                     | 0.56              |
| 18:B8:671:MET:HE1   | 18:B8:736:ALA:HB2   | 1.84                     | 0.56              |
| 18:B8:1439:LYS:HZ3  | 24:D32:1257:ASN:HB3 | 1.61                     | 0.56              |
| 19:4:250:ILE:HD11   | 20:E:163:ILE:CD1    | 2.22                     | 0.56              |
| 21:H16:228:LEU:HD11 | 23:J16:593:VAL:CG2  | 2.34                     | 0.56              |
| 24:D:308:ASN:CB     | 24:D16:753:ARG:NH2  | 2.68                     | 0.56              |
| 10:C32:1271:PHE:HE2 | 10:C32:1284:ASP:CA  | 2.18                     | 0.56              |
| 1:R:1145:LYS:HD2    | 1:R:1149:HIS:CE1    | 2.40                     | 0.56              |
| 1:R:1334:GLU:CG     | 10:C:1170:VAL:HG23  | 2.35                     | 0.56              |
| 3:N:208:LYS:HB3     | 3:N:239:ILE:CD1     | 2.34                     | 0.56              |
| 1:R8:1449:TRP:CH2   | 2:M8:161:ASP:C      | 2.78                     | 0.56              |
| 1:R8:1449:TRP:CH2   | 2:M8:161:ASP:N      | 2.73                     | 0.56              |
| 2:M8:217:ILE:HD11   | 3:N8:8:THR:HG21     | 1.87                     | 0.56              |
| 2:M8:342:VAL:CG1    | 2:M8:343:MET:N      | 2.59                     | 0.56              |
| 7:Q:219:GLY:O       | 7:Q:221:TRP:N       | 2.38                     | 0.56              |
| 5:P16:259:TYR:OH    | 5:P16:275:GLU:OE2   | 2.22                     | 0.56              |
| 5:P16:465:TYR:HE1   | 5:P16:482:TYR:CZ    | 2.24                     | 0.56              |
| 7:Q16:254:ALA:HB2   | 7:Q16:302:ILE:HD13  | 1.87                     | 0.56              |
| 7:Q16:266:LEU:HD21  | 7:Q16:302:ILE:HD12  | 1.87                     | 0.56              |
| 9:K:631:VAL:CG1     | 9:K:764:VAL:HB      | 2.27                     | 0.56              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K:923:ILE:HG22    | 9:K:929:ARG:HH21     | 1.70                     | 0.56              |
| 10:C16:75:GLN:HE21  | 10:C16:112:PRO:CG    | 2.16                     | 0.56              |
| 10:C16:244:ASN:HD22 | 10:C16:263:LEU:CD1   | 2.18                     | 0.56              |
| 10:C16:688:TRP:CZ2  | 10:C16:777:LEU:HD13  | 2.40                     | 0.56              |
| 10:C16:1335:ILE:O   | 10:C16:1336:ALA:C    | 2.48                     | 0.56              |
| 10:C24:325:MET:CE   | 10:C24:352:LEU:HD11  | 2.35                     | 0.56              |
| 11:A40:737:GLU:HG3  | 24:D32:871:ARG:NH2   | 2.07                     | 0.56              |
| 12:A:144:LYS:HE2    | 10:C:1821:VAL:HG11   | 1.86                     | 0.56              |
| 12:A:362:ARG:HG2    | 12:A:366:ARG:NH1     | 2.21                     | 0.56              |
| 12:A:557:LEU:HD23   | 12:A:561:ASP:HB3     | 1.85                     | 0.56              |
| 13:V:850:LEU:CD2    | 15:J:665:ILE:HD12    | 2.30                     | 0.56              |
| 10:C:853:GLY:C      | 10:C:856:PRO:HD2     | 2.30                     | 0.56              |
| 11:A16:445:ASN:ND2  | 17:F8:65:ARG:HH12    | 1.99                     | 0.56              |
| 11:A16:696:ILE:CD1  | 11:A16:728:ILE:CD1   | 2.82                     | 0.56              |
| 18:B:94:LEU:CD2     | 18:B:132:LEU:CD2     | 2.77                     | 0.56              |
| 18:B8:986:ALA:C     | 18:B8:988:SER:H      | 2.14                     | 0.56              |
| 18:B8:1505:MET:CE   | 18:B8:1518:VAL:CG2   | 2.84                     | 0.56              |
| 20:E:24:ILE:HB      | 20:E:25:PRO:HD3      | 1.88                     | 0.56              |
| 20:E:50:PHE:CZ      | 20:E:54:HIS:CD2      | 2.93                     | 0.56              |
| 21:H8:284:LEU:CD2   | 23:J8:650:GLN:HB3    | 2.36                     | 0.56              |
| 21:H16:194:VAL:HG13 | 21:H16:199:ASP:CB    | 2.34                     | 0.56              |
| 10:C32:565:ARG:HA   | 10:C32:568:TRP:CD2   | 2.41                     | 0.56              |
| 10:C32:761:VAL:CG2  | 10:C32:826:TYR:HA    | 2.35                     | 0.56              |
| 10:C32:1111:SER:OG  | 10:C32:1114:TYR:CD2  | 2.57                     | 0.56              |
| 10:C32:1246:SER:C   | 10:C32:1309:ARG:HH22 | 2.14                     | 0.56              |
| 12:A48:638:LEU:HA   | 12:A48:644:GLY:HA2   | 1.86                     | 0.56              |
| 2:M:202:LYS:HE2     | 2:M:206:SER:C        | 2.30                     | 0.56              |
| 2:M:211:MET:CE      | 3:N:280:ASN:HA       | 2.35                     | 0.56              |
| 1:R8:1124:TRP:CE3   | 1:R8:1170:LEU:O      | 2.59                     | 0.56              |
| 1:R8:1188:TYR:CZ    | 24:D40:1459:LEU:HD13 | 2.40                     | 0.56              |
| 1:R16:1269:LEU:CD1  | 5:P16:684:ARG:NE     | 2.59                     | 0.56              |
| 1:R16:1449:TRP:CH2  | 2:M16:161:ASP:N      | 2.73                     | 0.56              |
| 5:P:465:TYR:HE1     | 5:P:482:TYR:CZ       | 2.24                     | 0.56              |
| 7:Q:254:ALA:HB2     | 7:Q:302:ILE:HD13     | 1.87                     | 0.56              |
| 6:O8:69:TYR:CZ      | 6:O8:122:LEU:HB2     | 2.41                     | 0.56              |
| 7:Q8:266:LEU:HD21   | 7:Q8:302:ILE:HD12    | 1.87                     | 0.56              |
| 9:K:987:TYR:CE2     | 9:K:1016:PHE:HD2     | 2.23                     | 0.56              |
| 9:K:1230:LEU:CD2    | 9:K:1244:VAL:HG22    | 2.34                     | 0.56              |
| 10:C16:472:ASN:OD1  | 10:C16:473:PHE:N     | 2.39                     | 0.56              |
| 10:C16:1708:ARG:HE  | 10:C16:1733:ARG:NH1  | 2.03                     | 0.56              |
| 11:A24:156:MET:CB   | 11:A24:555:HIS:CD2   | 2.53                     | 0.56              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A24:468:VAL:CG2  | 24:D16:1103:LEU:HD11 | 2.13                     | 0.56              |
| 11:A24:587:VAL:CG2  | 11:A24:636:PHE:HE1   | 2.18                     | 0.56              |
| 10:C24:1340:PRO:HG2 | 10:C24:1746:GLY:CA   | 2.34                     | 0.56              |
| 10:C24:1340:PRO:CG  | 10:C24:1746:GLY:HA3  | 2.35                     | 0.56              |
| 10:C24:1796:LEU:HG  | 10:C24:1800:LEU:HD12 | 1.87                     | 0.56              |
| 13:V:745:LEU:HD13   | 15:J:557:ARG:HH12    | 1.61                     | 0.56              |
| 13:V:825:GLN:CA     | 14:W:707:LYS:NZ      | 2.68                     | 0.56              |
| 10:C:688:TRP:CZ2    | 10:C:777:LEU:HD13    | 2.40                     | 0.56              |
| 10:C:743:PHE:CE2    | 10:C:749:LEU:HD22    | 2.40                     | 0.56              |
| 10:C:1358:ASP:C     | 10:C:1360:GLN:H      | 2.14                     | 0.56              |
| 10:C8:761:VAL:CG2   | 10:C8:826:TYR:HA     | 2.35                     | 0.56              |
| 11:A16:90:PHE:CD2   | 18:B:1788:ILE:CG1    | 2.89                     | 0.56              |
| 11:A16:154:ILE:HA   | 11:A16:157:LEU:HD12  | 1.87                     | 0.56              |
| 17:F:69:SER:O       | 17:F:71:GLU:N        | 2.38                     | 0.56              |
| 11:A32:154:ILE:HA   | 11:A32:157:LEU:HD12  | 1.87                     | 0.56              |
| 18:B:472:SER:HA     | 18:B:584:ARG:NH1     | 2.21                     | 0.56              |
| 18:B:1137:ASP:OD1   | 18:B:1138:PRO:HD2    | 2.06                     | 0.56              |
| 18:B8:1234:MET:HB2  | 18:B8:1235:PRO:HD3   | 1.88                     | 0.56              |
| 22:I24:289:LEU:CD2  | 22:I24:296:ARG:HH12  | 2.17                     | 0.56              |
| 21:H16:154:VAL:HG13 | 21:H16:188:ARG:CG    | 2.35                     | 0.56              |
| 21:H16:260:ILE:HG23 | 23:J16:628:TYR:HB2   | 1.87                     | 0.56              |
| 21:H16:284:LEU:CD2  | 23:J16:650:GLN:HB3   | 2.36                     | 0.56              |
| 10:C32:510:TRP:N    | 10:C32:511:PRO:HD2   | 2.21                     | 0.56              |
| 10:C32:1796:LEU:HG  | 10:C32:1800:LEU:HD12 | 1.87                     | 0.56              |
| 2:M:421:LEU:HD11    | 8:L:346:TRP:HD1      | 1.63                     | 0.56              |
| 2:M8:202:LYS:HE2    | 2:M8:206:SER:C       | 2.30                     | 0.56              |
| 1:R16:1239:TRP:CE2  | 1:R16:1251:LEU:HD13  | 2.41                     | 0.56              |
| 9:K:621:ASN:ND2     | 9:K:683:GLN:OE1      | 2.39                     | 0.56              |
| 11:A24:362:ARG:NE   | 11:A24:366:ARG:HH22  | 2.03                     | 0.56              |
| 11:A40:107:GLN:NE2  | 21:H16:324:LEU:O     | 2.37                     | 0.56              |
| 12:A:634:ILE:HD13   | 12:A:678:LYS:HZ2     | 1.70                     | 0.56              |
| 13:V:762:LEU:O      | 13:V:766:VAL:HG23    | 2.05                     | 0.56              |
| 13:V:920:MET:HE3    | 14:W:797:ILE:HG21    | 1.88                     | 0.56              |
| 15:J:683:ILE:C      | 15:J:685:GLY:H       | 2.11                     | 0.56              |
| 10:C:60:LYS:HG2     | 10:C:77:ILE:HD11     | 1.87                     | 0.56              |
| 10:C8:847:ARG:CD    | 10:C8:903:ASN:OD1    | 2.53                     | 0.56              |
| 10:C8:853:GLY:C     | 10:C8:856:PRO:HD2    | 2.30                     | 0.56              |
| 10:C8:1058:GLU:O    | 10:C8:1059:ALA:C     | 2.46                     | 0.56              |
| 10:C8:1271:PHE:HE2  | 10:C8:1284:ASP:CA    | 2.19                     | 0.56              |
| 18:B:1515:LEU:HD21  | 18:B:1563:PHE:HB2    | 1.88                     | 0.56              |
| 18:B:1739:LEU:HD22  | 18:B:1777:LEU:HD22   | 1.88                     | 0.56              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B:1785:LYS:O     | 18:B:1787:LYS:N      | 2.39                     | 0.56              |
| 18:B8:624:ILE:O     | 18:B8:627:SER:OG     | 2.19                     | 0.56              |
| 18:B8:842:ASN:OD1   | 18:B8:899:LYS:NZ     | 2.39                     | 0.56              |
| 18:B8:1739:LEU:HD22 | 18:B8:1777:LEU:HD22  | 1.88                     | 0.56              |
| 20:E:407:LEU:CD1    | 20:E:462:THR:HG23    | 2.35                     | 0.56              |
| 20:E8:201:LEU:O     | 20:E8:203:TRP:N      | 2.39                     | 0.56              |
| 22:I8:289:LEU:CD2   | 22:I8:296:ARG:HH12   | 2.17                     | 0.56              |
| 21:H24:294:PRO:O    | 21:H24:300:ARG:NH2   | 2.38                     | 0.56              |
| 10:C32:565:ARG:NH1  | 10:C32:602:VAL:CG1   | 2.68                     | 0.56              |
| 12:A48:806:GLN:CG   | 12:A48:847:ARG:HH22  | 2.16                     | 0.56              |
| 2:M:257:VAL:CG2     | 2:M:274:VAL:HG21     | 2.35                     | 0.56              |
| 1:R16:1431:ARG:O    | 2:M16:177:VAL:CG1    | 2.54                     | 0.56              |
| 3:N16:256:LYS:HD2   | 3:N16:286:TRP:HH2    | 1.70                     | 0.56              |
| 5:P:259:TYR:OH      | 5:P:275:GLU:OE2      | 2.23                     | 0.56              |
| 5:P:291:LEU:CD1     | 5:P:299:CYS:SG       | 2.94                     | 0.56              |
| 7:Q:27:GLN:HB2      | 7:Q:341:GLN:OE1      | 2.06                     | 0.56              |
| 7:Q:236:HIS:HE1     | 7:Q:238:SER:OG       | 1.89                     | 0.56              |
| 5:P8:101:LEU:HD23   | 5:P8:133:TYR:CD1     | 2.40                     | 0.56              |
| 5:P8:675:LEU:HD12   | 5:P8:704:LEU:CD1     | 2.36                     | 0.56              |
| 7:Q16:124:PHE:CE1   | 7:Q16:125:TYR:CE2    | 2.80                     | 0.56              |
| 9:K:1055:THR:O      | 9:K:1057:GLU:N       | 2.39                     | 0.56              |
| 10:C16:1614:LEU:CD1 | 10:C16:1635:LEU:HD23 | 2.36                     | 0.56              |
| 11:A24:303:ALA:HB2  | 11:A24:321:ILE:HD11  | 1.87                     | 0.56              |
| 10:C24:510:TRP:N    | 10:C24:511:PRO:HD2   | 2.21                     | 0.56              |
| 10:C24:1234:ASP:OD1 | 10:C24:1302:LYS:NZ   | 2.25                     | 0.56              |
| 11:A40:743:ARG:HH22 | 24:D32:699:HIS:CG    | 2.23                     | 0.56              |
| 12:A:259:ILE:HG22   | 12:A:276:LEU:CD2     | 2.36                     | 0.56              |
| 10:C:8:VAL:CG2      | 10:C:133:THR:OG1     | 2.52                     | 0.56              |
| 10:C8:60:LYS:HG2    | 10:C8:77:ILE:HD11    | 1.87                     | 0.56              |
| 10:C8:663:ILE:HG22  | 10:C8:667:ILE:HG23   | 1.86                     | 0.56              |
| 10:C8:743:PHE:CE2   | 10:C8:749:LEU:HD22   | 2.40                     | 0.56              |
| 11:A16:154:ILE:CG2  | 18:B:1851:VAL:HG21   | 2.36                     | 0.56              |
| 11:A32:154:ILE:CG2  | 18:B8:1851:VAL:HG21  | 2.36                     | 0.56              |
| 18:B8:643:MET:HE2   | 18:B8:711:CYS:HB3    | 1.87                     | 0.56              |
| 18:B8:1799:VAL:C    | 18:B8:1801:GLY:H     | 2.13                     | 0.56              |
| 19:4:179:MET:O      | 20:E:416:LYS:HE3     | 2.05                     | 0.56              |
| 20:E:201:LEU:O      | 20:E:203:TRP:N       | 2.39                     | 0.56              |
| 20:E:432:ILE:HG22   | 20:E:434:TRP:CD1     | 2.40                     | 0.56              |
| 10:C32:278:ARG:NH1  | 10:C32:287:SER:CB    | 2.62                     | 0.56              |
| 10:C32:397:LEU:HD21 | 10:C32:444:LEU:HD21  | 1.88                     | 0.56              |
| 10:C32:1358:ASP:C   | 10:C32:1360:GLN:H    | 2.14                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A48:362:ARG:HG2  | 12:A48:366:ARG:NH1  | 2.21                     | 0.56              |
| 1:R16:526:ASN:HA    | 1:R16:529:HIS:HE1   | 1.64                     | 0.56              |
| 2:M16:202:LYS:HE2   | 2:M16:206:SER:C     | 2.31                     | 0.56              |
| 5:P:675:LEU:HD12    | 5:P:704:LEU:CD1     | 2.36                     | 0.56              |
| 5:P8:566:PHE:HZ     | 5:P8:597:GLY:C      | 2.13                     | 0.56              |
| 8:L16:1068:PHE:HD1  | 8:L16:1068:PHE:C    | 2.14                     | 0.56              |
| 9:K:879:CYS:HB2     | 9:K:900:TYR:HE2     | 1.71                     | 0.56              |
| 9:K:1133:ILE:HG21   | 9:K:1166:LEU:HD23   | 1.88                     | 0.56              |
| 9:K8:1065:GLU:C     | 9:K8:1067:VAL:N     | 2.64                     | 0.56              |
| 9:K8:1259:LYS:O     | 9:K8:1263:THR:OG1   | 2.20                     | 0.56              |
| 10:C16:719:PRO:C    | 10:C16:721:PHE:N    | 2.62                     | 0.56              |
| 10:C24:244:ASN:HD22 | 10:C24:263:LEU:CD1  | 2.18                     | 0.56              |
| 10:C24:397:LEU:HD21 | 10:C24:444:LEU:HD21 | 1.88                     | 0.56              |
| 10:C24:472:ASN:OD1  | 10:C24:473:PHE:N    | 2.39                     | 0.56              |
| 10:C24:565:ARG:HA   | 10:C24:568:TRP:CD2  | 2.41                     | 0.56              |
| 10:C24:586:PRO:CD   | 10:C24:650:ARG:HH12 | 2.10                     | 0.56              |
| 10:C24:1286:MET:CE  | 10:C24:1344:VAL:CG1 | 2.84                     | 0.56              |
| 10:C24:1395:GLY:O   | 10:C24:1400:LYS:HE3 | 2.06                     | 0.56              |
| 11:A40:259:ILE:HG22 | 11:A40:276:LEU:CD2  | 2.35                     | 0.56              |
| 11:A40:362:ARG:NE   | 11:A40:366:ARG:HH22 | 2.03                     | 0.56              |
| 12:A:302:GLN:HE21   | 12:A:324:ARG:NH1    | 1.97                     | 0.56              |
| 10:C:397:LEU:HD21   | 10:C:444:LEU:HD21   | 1.88                     | 0.56              |
| 10:C:520:TYR:OH     | 10:C:542:ASP:OD2    | 2.23                     | 0.56              |
| 10:C:761:VAL:CG2    | 10:C:826:TYR:HA     | 2.36                     | 0.56              |
| 10:C:1271:PHE:HE2   | 10:C:1284:ASP:CA    | 2.19                     | 0.56              |
| 10:C:1286:MET:CE    | 10:C:1344:VAL:CG1   | 2.84                     | 0.56              |
| 11:A16:303:ALA:HB2  | 11:A16:321:ILE:HD11 | 1.87                     | 0.56              |
| 11:A32:696:ILE:CD1  | 11:A32:728:ILE:CD1  | 2.82                     | 0.56              |
| 11:A32:706:SER:HB2  | 24:D32:1398:ARG:NE  | 2.19                     | 0.56              |
| 18:B:1152:ASP:OD1   | 18:B:1378:LYS:NZ    | 2.37                     | 0.56              |
| 18:B8:472:SER:HA    | 18:B8:584:ARG:NH1   | 2.21                     | 0.56              |
| 18:B8:1515:LEU:HD21 | 18:B8:1563:PHE:HB2  | 1.88                     | 0.56              |
| 19:4:250:ILE:CB     | 20:E:165:ARG:NH2    | 2.62                     | 0.56              |
| 20:E:448:LYS:HB2    | 20:E:451:ILE:HD12   | 1.88                     | 0.56              |
| 21:H8:260:ILE:HG23  | 23:J8:628:TYR:HB2   | 1.87                     | 0.56              |
| 21:H24:260:ILE:HG23 | 23:J24:628:TYR:HB2  | 1.87                     | 0.56              |
| 10:C32:445:MET:HE1  | 10:C32:462:PHE:CZ   | 2.41                     | 0.56              |
| 10:C32:853:GLY:C    | 10:C32:856:PRO:HD2  | 2.30                     | 0.56              |
| 10:C32:1389:ILE:O   | 10:C32:1393:SER:OG  | 2.23                     | 0.56              |
| 10:C32:1619:PRO:O   | 10:C32:1621:LYS:N   | 2.36                     | 0.56              |
| 1:R:1033:LYS:NZ     | 24:D:1432:THR:HG21  | 2.20                     | 0.56              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:R:1428:VAL:HG23   | 6:O:165:LYS:NZ       | 2.12                     | 0.56              |
| 5:P8:402:LEU:HD13   | 5:P8:433:LEU:HD13    | 1.88                     | 0.56              |
| 7:Q16:236:HIS:HE1   | 7:Q16:238:SER:OG     | 1.89                     | 0.56              |
| 8:L16:947:ASN:HB3   | 8:L16:1026:ARG:NH2   | 2.20                     | 0.56              |
| 10:C16:847:ARG:NH2  | 10:C16:910:SER:CB    | 2.59                     | 0.56              |
| 10:C16:1246:SER:C   | 10:C16:1309:ARG:HH22 | 2.14                     | 0.56              |
| 10:C24:168:ARG:HH12 | 10:C24:229:PRO:HA    | 1.70                     | 0.56              |
| 10:C24:1290:HIS:HD2 | 10:C24:1334:MET:HE2  | 1.66                     | 0.56              |
| 11:A40:28:SER:C     | 11:A40:30:PHE:H      | 2.14                     | 0.56              |
| 11:A40:375:ALA:N    | 11:A40:376:PRO:HD2   | 2.21                     | 0.56              |
| 11:A40:696:ILE:CD1  | 11:A40:728:ILE:CD1   | 2.82                     | 0.56              |
| 10:C:452:LEU:CD1    | 10:C:452:LEU:C       | 2.71                     | 0.56              |
| 10:C:561:ASN:OD1    | 10:C:562:PRO:CD      | 2.50                     | 0.56              |
| 10:C8:280:SER:C     | 10:C8:282:LYS:H      | 2.14                     | 0.56              |
| 10:C8:864:ALA:HB1   | 10:C8:914:LEU:HD11   | 1.87                     | 0.56              |
| 10:C8:1358:ASP:C    | 10:C8:1360:GLN:H     | 2.14                     | 0.56              |
| 11:A32:711:ARG:CD   | 24:D32:1398:ARG:HG2  | 2.35                     | 0.56              |
| 18:B:806:ILE:HD13   | 18:B:841:LEU:HD11    | 1.88                     | 0.56              |
| 18:B8:806:ILE:HD13  | 18:B8:841:LEU:HD11   | 1.88                     | 0.56              |
| 18:B8:1785:LYS:O    | 18:B8:1787:LYS:N     | 2.39                     | 0.56              |
| 19:4:423:PRO:HD2    | 19:4:441:PHE:HE1     | 1.69                     | 0.56              |
| 20:E8:350:GLU:HB3   | 20:E8:352:PHE:CD2    | 2.40                     | 0.56              |
| 21:H24:284:LEU:CD2  | 23:J24:650:GLN:HB3   | 2.36                     | 0.56              |
| 10:C32:280:SER:C    | 10:C32:282:LYS:H     | 2.14                     | 0.56              |
| 1:R:1033:LYS:HG3    | 24:D:1436:ARG:HE     | 1.68                     | 0.55              |
| 1:R:1124:TRP:CE3    | 1:R:1170:LEU:O       | 2.59                     | 0.55              |
| 1:R:1225:PHE:CE1    | 1:R:1247:PRO:HB3     | 2.40                     | 0.55              |
| 1:R:1473:HIS:CD2    | 6:O:160:LEU:HD13     | 2.41                     | 0.55              |
| 3:N:116:ILE:CG2     | 3:N:177:TYR:HE1      | 2.19                     | 0.55              |
| 3:N:263:TRP:NE1     | 3:N:279:GLY:HA2      | 2.18                     | 0.55              |
| 1:R8:1431:ARG:O     | 2:M8:177:VAL:CG1     | 2.54                     | 0.55              |
| 2:M8:166:THR:N      | 2:M8:169:THR:HG1     | 2.04                     | 0.55              |
| 2:M8:188:ARG:HB2    | 3:N8:264:ARG:NH1     | 2.20                     | 0.55              |
| 2:M8:202:LYS:HE2    | 2:M8:206:SER:O       | 2.06                     | 0.55              |
| 1:R16:1449:TRP:HZ2  | 2:M16:161:ASP:O      | 1.83                     | 0.55              |
| 2:M16:552:PHE:HZ    | 2:M16:559:PHE:CE2    | 2.17                     | 0.55              |
| 2:M16:844:VAL:HG13  | 4:T16:660:LEU:HD11   | 1.88                     | 0.55              |
| 5:P:109:ILE:HD13    | 14:W:18:PRO:HG2      | 1.77                     | 0.55              |
| 5:P:675:LEU:CD1     | 5:P:704:LEU:CD1      | 2.83                     | 0.55              |
| 5:P16:241:LEU:O     | 5:P16:369:TYR:OH     | 2.18                     | 0.55              |
| 9:K:798:LEU:CB      | 9:K:842:ILE:HD11     | 2.36                     | 0.55              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K:916:LYS:C       | 9:K:919:MET:HG2      | 2.29                     | 0.55              |
| 9:K8:1028:GLN:OE1   | 9:K8:1037:ALA:CA     | 2.47                     | 0.55              |
| 9:K16:975:MET:HG3   | 9:K16:985:PHE:HE1    | 1.70                     | 0.55              |
| 10:C16:11:VAL:HG21  | 10:C16:133:THR:HG23  | 1.87                     | 0.55              |
| 10:C16:397:LEU:HD21 | 10:C16:444:LEU:HD21  | 1.88                     | 0.55              |
| 10:C16:1395:GLY:O   | 10:C16:1400:LYS:HE3  | 2.06                     | 0.55              |
| 10:C16:1796:LEU:HG  | 10:C16:1800:LEU:HD12 | 1.87                     | 0.55              |
| 10:C24:60:LYS:HG2   | 10:C24:77:ILE:HD11   | 1.87                     | 0.55              |
| 10:C24:390:HIS:CG   | 10:C24:452:LEU:CG    | 2.87                     | 0.55              |
| 10:C24:1050:HIS:CE1 | 10:C24:1086:LYS:HZ1  | 2.19                     | 0.55              |
| 10:C24:1251:PHE:HZ  | 10:C24:1319:ARG:HH12 | 1.39                     | 0.55              |
| 10:C24:1285:VAL:HA  | 10:C24:1735:TYR:CE2  | 2.32                     | 0.55              |
| 10:C:169:GLN:O      | 10:C:173:THR:OG1     | 2.23                     | 0.55              |
| 10:C:565:ARG:HA     | 10:C:568:TRP:CD2     | 2.41                     | 0.55              |
| 10:C8:1337:LEU:HD23 | 16:A8:126:ARG:NH1    | 2.20                     | 0.55              |
| 10:C8:1619:PRO:O    | 10:C8:1621:LYS:N     | 2.36                     | 0.55              |
| 10:C8:1637:PHE:CD1  | 16:A8:136:LEU:HD11   | 2.41                     | 0.55              |
| 11:A16:437:LEU:CD1  | 11:A16:454:LYS:HZ3   | 2.17                     | 0.55              |
| 11:A16:823:VAL:HG12 | 11:A16:830:ILE:HD11  | 1.89                     | 0.55              |
| 11:A32:28:SER:C     | 11:A32:30:PHE:H      | 2.14                     | 0.55              |
| 18:B:273:MET:HG3    | 18:B:390:HIS:CD2     | 2.41                     | 0.55              |
| 18:B:786:ASP:CB     | 24:D16:1066:VAL:HG22 | 2.32                     | 0.55              |
| 21:H:154:VAL:HG13   | 21:H:188:ARG:CG      | 2.35                     | 0.55              |
| 21:H:260:ILE:HG23   | 23:J32:628:TYR:HB2   | 1.87                     | 0.55              |
| 23:J24:718:GLN:HE22 | 23:J24:737:TRP:HZ3   | 1.42                     | 0.55              |
| 1:R:1239:TRP:CE2    | 1:R:1251:LEU:HD13    | 2.41                     | 0.55              |
| 1:R:1335:ILE:HD11   | 10:C:1170:VAL:HG11   | 1.89                     | 0.55              |
| 1:R:1453:LYS:HZ1    | 10:C:616:GLN:HG3     | 1.70                     | 0.55              |
| 2:M:166:THR:N       | 2:M:169:THR:OG1      | 2.33                     | 0.55              |
| 1:R8:1239:TRP:CE2   | 1:R8:1251:LEU:HD13   | 2.41                     | 0.55              |
| 1:R16:1124:TRP:CE3  | 1:R16:1170:LEU:O     | 2.59                     | 0.55              |
| 7:Q:4:MET:HE2       | 7:Q:361:PRO:HB2      | 1.87                     | 0.55              |
| 5:P8:465:TYR:HE1    | 5:P8:482:TYR:CZ      | 2.24                     | 0.55              |
| 7:Q8:221:TRP:CH2    | 7:Q8:222:PHE:HE2     | 2.24                     | 0.55              |
| 9:K:621:ASN:OD1     | 9:K:622:VAL:N        | 2.40                     | 0.55              |
| 9:K8:798:LEU:CB     | 9:K8:842:ILE:HD11    | 2.36                     | 0.55              |
| 9:K8:1055:THR:O     | 9:K8:1057:GLU:N      | 2.39                     | 0.55              |
| 10:C16:615:GLU:HA   | 10:C16:619:LEU:HD12  | 1.88                     | 0.55              |
| 10:C16:1286:MET:CE  | 10:C16:1344:VAL:CG1  | 2.84                     | 0.55              |
| 10:C16:1358:ASP:C   | 10:C16:1361:LYS:H    | 2.13                     | 0.55              |
| 10:C24:615:GLU:HA   | 10:C24:619:LEU:HD12  | 1.88                     | 0.55              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1614:LEU:CD1 | 10:C24:1635:LEU:HD23 | 2.36                     | 0.55              |
| 11:A40:468:VAL:HG21 | 24:D32:1100:GLN:HB3  | 1.87                     | 0.55              |
| 12:A:240:GLU:O      | 12:A:242:THR:N       | 2.39                     | 0.55              |
| 12:A:362:ARG:NE     | 12:A:366:ARG:HH22    | 2.03                     | 0.55              |
| 14:W:680:ARG:HB3    | 15:J:603:LEU:HD21    | 1.88                     | 0.55              |
| 10:C:758:GLN:NE2    | 10:C:819:GLN:CG      | 2.69                     | 0.55              |
| 10:C:1395:GLY:O     | 10:C:1400:LYS:HE3    | 2.06                     | 0.55              |
| 10:C8:453:LEU:CD2   | 10:C8:459:LEU:CG     | 2.82                     | 0.55              |
| 10:C8:510:TRP:N     | 10:C8:511:PRO:HD2    | 2.21                     | 0.55              |
| 10:C8:1009:GLN:C    | 10:C8:1192:ARG:NH2   | 2.60                     | 0.55              |
| 11:A32:303:ALA:HB2  | 11:A32:321:ILE:HD11  | 1.87                     | 0.55              |
| 18:B:842:ASN:OD1    | 18:B:899:LYS:NZ      | 2.39                     | 0.55              |
| 18:B8:514:THR:HG23  | 18:B8:549:TRP:HZ3    | 1.68                     | 0.55              |
| 18:B8:712:PRO:HG2   | 18:B8:759:MET:HE1    | 0.60                     | 0.55              |
| 21:H24:193:LEU:HD21 | 21:H24:195:GLN:NE2   | 2.15                     | 0.55              |
| 10:C32:1212:GLU:OE1 | 12:A48:109:HIS:NE2   | 2.26                     | 0.55              |
| 10:C32:1340:PRO:CG  | 10:C32:1746:GLY:HA3  | 2.35                     | 0.55              |
| 10:C32:1614:LEU:CD1 | 10:C32:1635:LEU:HD23 | 2.36                     | 0.55              |
| 12:A48:224:PHE:O    | 12:A48:226:PRO:HD3   | 2.04                     | 0.55              |
| 12:A48:560:MET:HE2  | 12:A48:615:GLN:NE2   | 1.97                     | 0.55              |
| 2:M:173:SER:OG      | 3:N:234:GLN:NE2      | 2.31                     | 0.55              |
| 2:M8:257:VAL:HG23   | 2:M8:274:VAL:CG2     | 2.36                     | 0.55              |
| 2:M8:417:ARG:HG3    | 8:L8:298:PHE:CD2     | 2.42                     | 0.55              |
| 2:M8:537:ILE:CG1    | 2:M8:558:MET:HE3     | 2.36                     | 0.55              |
| 3:N8:208:LYS:HB3    | 3:N8:239:ILE:CD1     | 2.34                     | 0.55              |
| 2:M16:188:ARG:HB2   | 3:N16:264:ARG:NH1    | 2.20                     | 0.55              |
| 2:M16:257:VAL:HG23  | 2:M16:274:VAL:CG2    | 2.36                     | 0.55              |
| 2:M16:342:VAL:CG1   | 2:M16:343:MET:H      | 1.92                     | 0.55              |
| 5:P:600:PHE:CZ      | 5:P:638:SER:O        | 2.59                     | 0.55              |
| 5:P8:12:GLU:HB2     | 5:P8:78:GLY:HA3      | 1.88                     | 0.55              |
| 7:Q8:236:HIS:HE1    | 7:Q8:238:SER:OG      | 1.89                     | 0.55              |
| 7:Q16:97:PRO:HD2    | 7:Q16:113:ILE:O      | 2.06                     | 0.55              |
| 7:Q16:219:GLY:O     | 7:Q16:221:TRP:N      | 2.38                     | 0.55              |
| 9:K:649:MET:HB3     | 9:K:704:ARG:HH22     | 1.54                     | 0.55              |
| 9:K:774:LEU:O       | 9:K:778:LEU:HB2      | 2.05                     | 0.55              |
| 9:K8:828:PRO:CB     | 9:K8:830:HIS:CE1     | 2.89                     | 0.55              |
| 10:C16:510:TRP:N    | 10:C16:511:PRO:HD2   | 2.21                     | 0.55              |
| 10:C16:667:ILE:CG2  | 10:C16:669:GLY:C     | 2.68                     | 0.55              |
| 10:C16:1058:GLU:O   | 10:C16:1059:ALA:C    | 2.46                     | 0.55              |
| 10:C16:1337:LEU:CD2 | 11:A24:126:ARG:HH11  | 2.20                     | 0.55              |
| 10:C24:1619:PRO:O   | 10:C24:1621:LYS:N    | 2.36                     | 0.55              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:V:783:TRP:CZ2     | 14:W:671:GLU:HG3     | 2.36                     | 0.55              |
| 14:W:586:ILE:HD12    | 15:J:572:ASP:HB2     | 1.82                     | 0.55              |
| 18:B:241:TYR:HB2     | 18:B:271:LEU:CD2     | 2.32                     | 0.55              |
| 18:B:428:GLN:HG3     | 18:B:584:ARG:CZ      | 2.11                     | 0.55              |
| 20:E8:350:GLU:C      | 20:E8:352:PHE:N      | 2.64                     | 0.55              |
| 21:H:194:VAL:HG13    | 21:H:199:ASP:CB      | 2.34                     | 0.55              |
| 21:H:284:LEU:CD2     | 23:J32:650:GLN:HB3   | 2.36                     | 0.55              |
| 21:H:294:PRO:O       | 21:H:300:ARG:NH2     | 2.38                     | 0.55              |
| 22:I:131:ARG:CG      | 23:J32:557:ARG:HH22  | 2.11                     | 0.55              |
| 23:J32:734:PRO:O     | 23:J32:735:LYS:C     | 2.46                     | 0.55              |
| 23:J16:718:GLN:HE22  | 23:J16:737:TRP:HZ3   | 1.43                     | 0.55              |
| 10:C32:75:GLN:HE21   | 10:C32:112:PRO:CG    | 2.16                     | 0.55              |
| 10:C32:1286:MET:CE   | 10:C32:1344:VAL:CG1  | 2.84                     | 0.55              |
| 1:R:979:GLN:CG       | 24:D:1438:ALA:HB3    | 2.36                     | 0.55              |
| 1:R:1428:VAL:HG21    | 6:O:165:LYS:HZ2      | 1.62                     | 0.55              |
| 6:O:130:ASP:O        | 6:O:166:PRO:HG2      | 2.07                     | 0.55              |
| 7:Q:97:PRO:HD2       | 7:Q:113:ILE:O        | 2.06                     | 0.55              |
| 7:Q:265:VAL:HG11     | 7:Q:271:ALA:HB1      | 1.89                     | 0.55              |
| 5:P8:96:VAL:CG1      | 5:P8:481:ILE:HD13    | 2.31                     | 0.55              |
| 5:P8:610:SER:C       | 5:P8:629:ARG:HH21    | 2.06                     | 0.55              |
| 5:P8:634:MET:HG3     | 5:P8:671:MET:SD      | 2.47                     | 0.55              |
| 7:Q8:27:GLN:HB2      | 7:Q8:341:GLN:OE1     | 2.06                     | 0.55              |
| 5:P16:12:GLU:HB2     | 5:P16:78:GLY:HA3     | 1.88                     | 0.55              |
| 6:O16:69:TYR:CZ      | 6:O16:122:LEU:HB2    | 2.41                     | 0.55              |
| 7:Q16:221:TRP:CH2    | 7:Q16:222:PHE:HE2    | 2.24                     | 0.55              |
| 8:L16:1031:PRO:HA    | 8:L16:1068:PHE:CZ    | 2.39                     | 0.55              |
| 9:K8:707:GLN:OE1     | 9:K8:761:TYR:OH      | 2.22                     | 0.55              |
| 10:C16:60:LYS:HG2    | 10:C16:77:ILE:HD11   | 1.87                     | 0.55              |
| 10:C16:229:PRO:HG2   | 10:C16:270:THR:HG23  | 1.87                     | 0.55              |
| 10:C16:1340:PRO:CG   | 10:C16:1746:GLY:HA3  | 2.35                     | 0.55              |
| 10:C16:1449:GLU:OE1  | 24:D8:1151:SER:CA    | 2.55                     | 0.55              |
| 11:A24:803:PRO:HB3   | 24:D8:1401:LEU:CG    | 2.32                     | 0.55              |
| 10:C24:11:VAL:HG21   | 10:C24:133:THR:HG23  | 1.87                     | 0.55              |
| 10:C24:445:MET:HE1   | 10:C24:462:PHE:CZ    | 2.41                     | 0.55              |
| 10:C24:643:LEU:CD2   | 10:C24:675:ASP:CG    | 2.69                     | 0.55              |
| 10:C24:1246:SER:C    | 10:C24:1309:ARG:HH22 | 2.14                     | 0.55              |
| 10:C24:1477:GLN:HG2  | 24:D24:1407:PHE:CG   | 2.42                     | 0.55              |
| 10:C24:1682:VAL:HG22 | 10:C24:1758:LEU:CD2  | 2.36                     | 0.55              |
| 12:A:136:LEU:HD11    | 10:C:1637:PHE:CD1    | 2.41                     | 0.55              |
| 10:C:280:SER:C       | 10:C:282:LYS:H       | 2.14                     | 0.55              |
| 10:C:510:TRP:N       | 10:C:511:PRO:HD2     | 2.21                     | 0.55              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:1109:VAL:HG12   | 10:C:1109:VAL:O      | 2.07                     | 0.55              |
| 10:C:1154:TRP:CZ2    | 10:C:1158:HIS:CD2    | 2.95                     | 0.55              |
| 10:C8:472:ASN:OD1    | 10:C8:473:PHE:N      | 2.39                     | 0.55              |
| 10:C8:565:ARG:HA     | 10:C8:568:TRP:CD2    | 2.41                     | 0.55              |
| 10:C8:1395:GLY:O     | 10:C8:1400:LYS:HE3   | 2.06                     | 0.55              |
| 11:A32:362:ARG:HG2   | 11:A32:366:ARG:NH1   | 2.21                     | 0.55              |
| 11:A32:362:ARG:NE    | 11:A32:366:ARG:HH22  | 2.03                     | 0.55              |
| 11:A32:823:VAL:HG12  | 11:A32:830:ILE:HD11  | 1.89                     | 0.55              |
| 18:B:230:ASN:OD1     | 18:B:233:ARG:HB2     | 2.06                     | 0.55              |
| 18:B:1434:VAL:HG13   | 18:B:1458:LEU:HD22   | 1.87                     | 0.55              |
| 18:B:1700:LEU:CD2    | 18:B:1833:PHE:CD2    | 2.89                     | 0.55              |
| 18:B8:957:ALA:HA     | 18:B8:964:LEU:HD22   | 1.88                     | 0.55              |
| 18:B8:1222:TYR:HB3   | 18:B8:1233:LEU:CD2   | 2.37                     | 0.55              |
| 18:B8:1390:LEU:HD11  | 18:B8:1404:LEU:CD1   | 2.36                     | 0.55              |
| 19:4:345:GLU:HB3     | 19:4:349:LEU:HD12    | 1.88                     | 0.55              |
| 21:H24:253:ARG:NE    | 23:J24:621:GLU:OE2   | 2.38                     | 0.55              |
| 10:C32:1358:ASP:C    | 10:C32:1361:LYS:H    | 2.13                     | 0.55              |
| 10:C32:1527:ARG:HH21 | 10:C32:1580:GLU:CD   | 2.14                     | 0.55              |
| 10:C32:1682:VAL:HG22 | 10:C32:1758:LEU:CD2  | 2.37                     | 0.55              |
| 12:A48:362:ARG:NE    | 12:A48:366:ARG:HH22  | 2.03                     | 0.55              |
| 1:R:1112:LYS:NZ      | 1:R:1156:GLU:OE1     | 2.29                     | 0.55              |
| 2:M:519:TYR:CE2      | 2:M:520:ILE:HG13     | 2.42                     | 0.55              |
| 2:M:614:TYR:CZ       | 2:M:618:HIS:CE1      | 2.95                     | 0.55              |
| 5:P:106:ARG:HH22     | 5:P:462:ARG:HH12     | 1.53                     | 0.55              |
| 6:O:133:LEU:HD22     | 6:O:189:LEU:HD22     | 1.87                     | 0.55              |
| 5:P8:14:VAL:HG22     | 5:P8:419:SER:OG      | 2.07                     | 0.55              |
| 6:O8:54:VAL:CG1      | 6:O8:85:TRP:HE1      | 2.15                     | 0.55              |
| 6:O8:133:LEU:HD22    | 6:O8:189:LEU:HD22    | 1.87                     | 0.55              |
| 7:Q8:97:PRO:HD2      | 7:Q8:113:ILE:O       | 2.06                     | 0.55              |
| 7:Q16:98:MET:HG2     | 7:Q16:112:MET:HG2    | 1.89                     | 0.55              |
| 7:Q16:147:GLU:OE1    | 7:Q16:159:VAL:HG11   | 2.07                     | 0.55              |
| 7:Q16:211:GLY:O      | 7:Q16:212:GLU:CG     | 2.54                     | 0.55              |
| 10:C16:1527:ARG:HH21 | 10:C16:1580:GLU:CD   | 2.14                     | 0.55              |
| 10:C16:1637:PHE:CD1  | 11:A24:136:LEU:HD11  | 2.41                     | 0.55              |
| 11:A24:28:SER:C      | 11:A24:30:PHE:H      | 2.14                     | 0.55              |
| 11:A24:240:GLU:O     | 11:A24:242:THR:N     | 2.40                     | 0.55              |
| 11:A24:259:ILE:HG22  | 11:A24:276:LEU:CD2   | 2.35                     | 0.55              |
| 10:C24:18:THR:CG2    | 10:C24:883:GLU:HG2   | 2.36                     | 0.55              |
| 10:C24:280:SER:C     | 10:C24:282:LYS:H     | 2.14                     | 0.55              |
| 10:C24:1637:PHE:CD1  | 11:A40:136:LEU:HD11  | 2.41                     | 0.55              |
| 11:A40:803:PRO:CA    | 24:D24:1401:LEU:HD12 | 2.32                     | 0.55              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:864:ALA:HB1     | 10:C:914:LEU:HD11    | 1.87                     | 0.55              |
| 10:C:1708:ARG:HE     | 10:C:1733:ARG:NH1    | 2.03                     | 0.55              |
| 11:A16:11:THR:CG2    | 22:I:162:GLN:NE2     | 2.67                     | 0.55              |
| 11:A16:28:SER:C      | 11:A16:30:PHE:H      | 2.14                     | 0.55              |
| 11:A32:153:ARG:NH1   | 18:B8:1846:GLU:OE1   | 2.38                     | 0.55              |
| 11:A32:467:SER:O     | 11:A32:469:VAL:N     | 2.40                     | 0.55              |
| 18:B:609:TYR:CD2     | 18:B:609:TYR:C       | 2.85                     | 0.55              |
| 18:B:1080:LEU:HD23   | 18:B:1334:LEU:HD11   | 1.89                     | 0.55              |
| 18:B:1222:TYR:HB3    | 18:B:1233:LEU:CD2    | 2.36                     | 0.55              |
| 18:B8:475:GLU:OE2    | 18:B8:588:PHE:CZ     | 2.59                     | 0.55              |
| 19:4:50:THR:O        | 19:4:52:SER:N        | 2.38                     | 0.55              |
| 20:E:252:LYS:HE2     | 20:E:297:TRP:NE1     | 2.22                     | 0.55              |
| 20:E:350:GLU:HG2     | 20:E:352:PHE:CE2     | 2.40                     | 0.55              |
| 20:E:353:ILE:CD1     | 20:E:413:PHE:CE2     | 2.76                     | 0.55              |
| 20:E8:124:LEU:HD23   | 20:E8:129:PHE:CE1    | 2.42                     | 0.55              |
| 23:J24:682:ALA:C     | 23:J24:684:ASP:H     | 2.15                     | 0.55              |
| 10:C32:1002:LEU:CD1  | 10:C32:1019:ARG:NH1  | 2.64                     | 0.55              |
| 10:C32:1340:PRO:HG2  | 10:C32:1746:GLY:CA   | 2.34                     | 0.55              |
| 2:M:507:LEU:CD2      | 2:M:514:TRP:CE3      | 2.90                     | 0.55              |
| 2:M8:847:PHE:CD1     | 4:T8:656:TRP:HE3     | 2.21                     | 0.55              |
| 2:M16:225:ASP:HB2    | 2:M16:606:GLN:NE2    | 2.20                     | 0.55              |
| 5:P:220:GLU:CD       | 5:P:232:ARG:NH1      | 2.62                     | 0.55              |
| 6:O:69:TYR:CZ        | 6:O:122:LEU:HB2      | 2.41                     | 0.55              |
| 7:Q16:27:GLN:HB2     | 7:Q16:341:GLN:OE1    | 2.06                     | 0.55              |
| 9:K:1019:ARG:HB3     | 9:K:1059:ARG:NH1     | 2.20                     | 0.55              |
| 9:K8:751:LEU:HD21    | 9:K8:754:ARG:HH11    | 1.68                     | 0.55              |
| 9:K16:912:TYR:CB     | 9:K16:957:ILE:HD11   | 2.36                     | 0.55              |
| 10:C16:172:ILE:HG23  | 10:C16:240:ILE:HD12  | 1.89                     | 0.55              |
| 10:C24:557:VAL:CG2   | 10:C24:565:ARG:NH2   | 2.45                     | 0.55              |
| 10:C24:1424:GLN:HE21 | 10:C24:1478:VAL:HG13 | 1.71                     | 0.55              |
| 14:W:711:ARG:CZ      | 10:C8:1606:GLY:CA    | 2.82                     | 0.55              |
| 10:C:11:VAL:HG21     | 10:C:133:THR:HG23    | 1.87                     | 0.55              |
| 10:C:275:ALA:CB      | 10:C:326:LEU:HD12    | 2.37                     | 0.55              |
| 10:C:1527:ARG:HH21   | 10:C:1580:GLU:CD     | 2.14                     | 0.55              |
| 10:C:1535:LEU:CB     | 10:C:1548:ILE:HD13   | 2.37                     | 0.55              |
| 10:C8:653:TYR:N      | 10:C8:654:PRO:HD3    | 2.22                     | 0.55              |
| 10:C8:1612:SER:O     | 10:C8:1616:ILE:HG13  | 2.07                     | 0.55              |
| 11:A16:638:LEU:HA    | 11:A16:644:GLY:HA2   | 1.86                     | 0.55              |
| 11:A32:122:LYS:NZ    | 18:B8:1757:GLU:CD    | 2.65                     | 0.55              |
| 11:A32:806:GLN:CG    | 11:A32:847:ARG:HH22  | 2.16                     | 0.55              |
| 18:B8:90:ILE:CD1     | 18:B8:105:VAL:HG22   | 2.36                     | 0.55              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B8:273:MET:HG3    | 18:B8:390:HIS:CD2   | 2.41                     | 0.55              |
| 18:B8:1911:LEU:CA    | 18:B8:1960:LEU:CD1  | 2.85                     | 0.55              |
| 19:4:232:TYR:CE2     | 19:4:233:ASP:OD1    | 2.60                     | 0.55              |
| 20:E:52:VAL:HG11     | 20:E:121:VAL:CG2    | 2.33                     | 0.55              |
| 20:E:124:LEU:HD23    | 20:E:129:PHE:CE1    | 2.42                     | 0.55              |
| 20:E:473:LEU:HD13    | 20:E:514:PHE:HB3    | 1.89                     | 0.55              |
| 19:48:345:GLU:HB3    | 19:48:349:LEU:HD12  | 1.88                     | 0.55              |
| 22:I8:328:TYR:CE1    | 23:J8:717:ILE:HG21  | 2.42                     | 0.55              |
| 21:H24:312:GLN:NE2   | 21:H24:316:ILE:HD11 | 2.22                     | 0.55              |
| 21:H16:179:GLU:O     | 21:H16:186:ARG:NH2  | 2.40                     | 0.55              |
| 22:I16:328:TYR:CE1   | 23:J16:717:ILE:HG21 | 2.42                     | 0.55              |
| 24:D40:1127:ARG:HA   | 24:D40:1127:ARG:NE  | 2.21                     | 0.55              |
| 10:C32:472:ASN:OD1   | 10:C32:473:PHE:N    | 2.39                     | 0.55              |
| 1:R:1290:ILE:CG1     | 10:C:605:GLU:OE2    | 2.54                     | 0.55              |
| 2:M:257:VAL:HG23     | 2:M:274:VAL:CG2     | 2.36                     | 0.55              |
| 2:M:820:LEU:HD23     | 4:T:656:TRP:CZ2     | 2.42                     | 0.55              |
| 2:M8:217:ILE:HD12    | 3:N8:8:THR:CG2      | 2.37                     | 0.55              |
| 2:M8:820:LEU:HD23    | 4:T8:656:TRP:CZ2    | 2.42                     | 0.55              |
| 5:P:233:TYR:CE1      | 5:P:237:MET:CE      | 2.90                     | 0.55              |
| 6:O:179:LYS:O        | 6:O:180:GLY:O       | 2.25                     | 0.55              |
| 5:P8:291:LEU:CD1     | 5:P8:299:CYS:SG     | 2.94                     | 0.55              |
| 7:Q8:147:GLU:OE1     | 7:Q8:159:VAL:HG11   | 2.07                     | 0.55              |
| 6:O16:90:GLU:CD      | 6:O16:98:LYS:HZ2    | 2.15                     | 0.55              |
| 6:O16:179:LYS:O      | 6:O16:180:GLY:O     | 2.25                     | 0.55              |
| 9:K:1056:VAL:HG21    | 9:K:1059:ARG:NH2    | 2.22                     | 0.55              |
| 9:K8:879:CYS:HB2     | 9:K8:900:TYR:HE2    | 1.71                     | 0.55              |
| 9:K8:1198:LEU:HD11   | 9:K8:1267:LEU:CD2   | 2.28                     | 0.55              |
| 9:K8:1230:LEU:HD23   | 9:K8:1244:VAL:HG23  | 1.88                     | 0.55              |
| 10:C16:286:ILE:CG2   | 10:C16:292:PHE:CD1  | 2.87                     | 0.55              |
| 10:C16:761:VAL:CG2   | 10:C16:826:TYR:HA   | 2.36                     | 0.55              |
| 10:C16:1109:VAL:HG12 | 10:C16:1109:VAL:O   | 2.07                     | 0.55              |
| 11:A24:445:ASN:ND2   | 17:F:65:ARG:HH12    | 1.99                     | 0.55              |
| 11:A24:645:GLU:CG    | 24:D16:867:ASP:CG   | 2.51                     | 0.55              |
| 10:C24:169:GLN:O     | 10:C24:173:THR:OG1  | 2.23                     | 0.55              |
| 11:A40:240:GLU:O     | 11:A40:242:THR:N    | 2.40                     | 0.55              |
| 13:V:832:LEU:HD21    | 13:V:836:LEU:HB3    | 1.89                     | 0.55              |
| 10:C:172:ILE:HG23    | 10:C:240:ILE:HD12   | 1.89                     | 0.55              |
| 10:C:472:ASN:OD1     | 10:C:473:PHE:N      | 2.39                     | 0.55              |
| 10:C:653:TYR:N       | 10:C:654:PRO:HD3    | 2.22                     | 0.55              |
| 10:C:983:SER:OG      | 10:C:1040:HIS:CD2   | 2.59                     | 0.55              |
| 10:C:1058:GLU:O      | 10:C:1059:ALA:C     | 2.46                     | 0.55              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C8:397:LEU:HD21   | 10:C8:444:LEU:HD21  | 1.88                     | 0.55              |
| 10:C8:1465:LEU:HD23  | 16:A8:124:ASN:OD1   | 2.07                     | 0.55              |
| 10:C8:1527:ARG:HH21  | 10:C8:1580:GLU:CD   | 2.14                     | 0.55              |
| 11:A16:122:LYS:CD    | 18:B:1757:GLU:OE1   | 2.55                     | 0.55              |
| 11:A16:362:ARG:NE    | 11:A16:366:ARG:HH22 | 2.03                     | 0.55              |
| 11:A16:386:GLY:O     | 11:A16:459:ARG:CZ   | 2.53                     | 0.55              |
| 11:A32:259:ILE:HG22  | 11:A32:276:LEU:CD2  | 2.36                     | 0.55              |
| 18:B:1911:LEU:CA     | 18:B:1960:LEU:HD11  | 2.37                     | 0.55              |
| 18:B8:609:TYR:CD2    | 18:B8:609:TYR:C     | 2.85                     | 0.55              |
| 18:B8:1080:LEU:HD23  | 18:B8:1334:LEU:HD11 | 1.89                     | 0.55              |
| 20:E:355:PRO:C       | 20:E:454:MET:HE1    | 2.32                     | 0.55              |
| 19:48:56:GLU:C       | 19:48:58:GLU:N      | 2.65                     | 0.55              |
| 19:48:126:ARG:NH1    | 19:48:134:LYS:O     | 2.36                     | 0.55              |
| 19:48:232:TYR:CE2    | 19:48:233:ASP:OD1   | 2.60                     | 0.55              |
| 22:I:328:TYR:CE1     | 23:J32:717:ILE:HG21 | 2.42                     | 0.55              |
| 23:J32:678:GLY:O     | 23:J32:680:LEU:N    | 2.40                     | 0.55              |
| 21:H8:228:LEU:HD11   | 23:J8:593:VAL:CG2   | 2.34                     | 0.55              |
| 21:H16:294:PRO:O     | 21:H16:300:ARG:NH2  | 2.38                     | 0.55              |
| 10:C32:1109:VAL:HG12 | 10:C32:1109:VAL:O   | 2.07                     | 0.55              |
| 2:M8:507:LEU:CD2     | 2:M8:514:TRP:CE3    | 2.90                     | 0.55              |
| 2:M8:614:TYR:CZ      | 2:M8:618:HIS:CE1    | 2.95                     | 0.55              |
| 5:P:644:TRP:HB2      | 5:P:678:LEU:HD11    | 1.87                     | 0.55              |
| 7:Q8:211:GLY:O       | 7:Q8:212:GLU:CG     | 2.55                     | 0.55              |
| 5:P16:233:TYR:CE1    | 5:P16:237:MET:CE    | 2.90                     | 0.55              |
| 7:Q16:309:SER:OG     | 7:Q16:311:ASP:OD1   | 2.20                     | 0.55              |
| 8:L16:1066:THR:HB    | 9:K16:1285:GLU:O    | 2.06                     | 0.55              |
| 9:K8:621:ASN:ND2     | 9:K8:683:GLN:OE1    | 2.39                     | 0.55              |
| 9:K8:1282:SER:C      | 9:K8:1284:MET:N     | 2.64                     | 0.55              |
| 10:C16:280:SER:C     | 10:C16:282:LYS:H    | 2.14                     | 0.55              |
| 10:C16:653:TYR:N     | 10:C16:654:PRO:HD3  | 2.22                     | 0.55              |
| 10:C16:768:ARG:HH22  | 10:C16:775:LYS:HG2  | 1.68                     | 0.55              |
| 10:C16:1389:ILE:O    | 10:C16:1393:SER:OG  | 2.23                     | 0.55              |
| 11:A24:467:SER:O     | 11:A24:469:VAL:N    | 2.40                     | 0.55              |
| 10:C24:1058:GLU:O    | 10:C24:1059:ALA:C   | 2.46                     | 0.55              |
| 10:C24:1378:LYS:HA   | 10:C24:1381:ALA:HB2 | 1.89                     | 0.55              |
| 10:C24:1527:ARG:HH21 | 10:C24:1580:GLU:CD  | 2.14                     | 0.55              |
| 10:C24:1541:PHE:CE1  | 10:C24:1649:LYS:CD  | 2.88                     | 0.55              |
| 11:A40:467:SER:O     | 11:A40:469:VAL:N    | 2.40                     | 0.55              |
| 10:C:1682:VAL:HG22   | 10:C:1758:LEU:CD2   | 2.36                     | 0.55              |
| 11:A16:515:LEU:HD21  | 11:A16:565:GLU:OE2  | 2.07                     | 0.55              |
| 18:B:191:PHE:CE2     | 18:B:192:PRO:O      | 2.60                     | 0.55              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 18:B:475:GLU:OE2   | 18:B:588:PHE:CZ      | 2.59                     | 0.55              |
| 18:B:1112:LYS:CE   | 21:H:327:SER:CB      | 2.84                     | 0.55              |
| 18:B:1579:ASN:HD21 | 24:D16:1403:LEU:HD22 | 1.71                     | 0.55              |
| 20:E8:24:ILE:HB    | 20:E8:25:PRO:HD3     | 1.88                     | 0.55              |
| 20:E8:252:LYS:HE2  | 20:E8:297:TRP:NE1    | 2.22                     | 0.55              |
| 20:E8:350:GLU:HG2  | 20:E8:352:PHE:CE2    | 2.40                     | 0.55              |
| 23:J32:682:ALA:C   | 23:J32:684:ASP:H     | 2.15                     | 0.55              |
| 24:D40:873:ARG:HD2 | 24:D40:884:ASP:CG    | 2.31                     | 0.55              |
| 10:C32:169:GLN:O   | 10:C32:173:THR:OG1   | 2.23                     | 0.55              |
| 10:C32:1395:GLY:O  | 10:C32:1400:LYS:HE3  | 2.06                     | 0.55              |
| 12:A48:240:GLU:O   | 12:A48:242:THR:N     | 2.39                     | 0.55              |
| 12:A48:257:GLN:NE2 | 12:A48:263:ASP:CG    | 2.60                     | 0.55              |
| 12:A48:375:ALA:N   | 12:A48:376:PRO:HD2   | 2.21                     | 0.55              |
| 12:A48:524:GLU:OE2 | 12:A48:530:TYR:CD2   | 2.60                     | 0.55              |
| 1:R8:1190:VAL:HG22 | 24:D40:1456:GLU:HB3  | 1.87                     | 0.55              |
| 1:R8:1466:LYS:HD2  | 6:O8:160:LEU:CD2     | 2.37                     | 0.55              |
| 2:M16:217:ILE:HD12 | 3:N16:8:THR:CG2      | 2.37                     | 0.55              |
| 2:M16:627:TYR:CG   | 3:N16:166:ALA:O      | 2.58                     | 0.55              |
| 2:M16:820:LEU:HD23 | 4:T16:656:TRP:CZ2    | 2.42                     | 0.55              |
| 3:N16:263:TRP:NE1  | 3:N16:279:GLY:HA2    | 2.18                     | 0.55              |
| 5:P:14:VAL:HG22    | 5:P:419:SER:OG       | 2.07                     | 0.55              |
| 5:P:634:MET:HG3    | 5:P:671:MET:SD       | 2.47                     | 0.55              |
| 7:Q:98:MET:HG2     | 7:Q:112:MET:HG2      | 1.89                     | 0.55              |
| 7:Q16:265:VAL:HG11 | 7:Q16:271:ALA:HB1    | 1.89                     | 0.55              |
| 8:L8:605:MET:CG    | 8:L8:631:LEU:HD13    | 2.36                     | 0.55              |
| 8:L8:608:PHE:CE1   | 8:L8:635:MET:HG2     | 2.41                     | 0.55              |
| 9:K:806:LEU:HD12   | 9:K:874:VAL:HG11     | 1.88                     | 0.55              |
| 9:K8:1207:PHE:HZ   | 9:K8:1271:GLU:OE2    | 1.88                     | 0.55              |
| 10:C16:18:THR:CG2  | 10:C16:883:GLU:HG2   | 2.36                     | 0.55              |
| 10:C16:854:LEU:CD2 | 10:C16:911:ILE:HD11  | 2.33                     | 0.55              |
| 10:C16:1378:LYS:HA | 10:C16:1381:ALA:HB2  | 1.89                     | 0.55              |
| 11:A24:362:ARG:CG  | 11:A24:366:ARG:CZ    | 2.85                     | 0.55              |
| 11:A24:375:ALA:N   | 11:A24:376:PRO:HD2   | 2.21                     | 0.55              |
| 10:C24:75:GLN:HE21 | 10:C24:112:PRO:CG    | 2.16                     | 0.55              |
| 10:C24:229:PRO:HG2 | 10:C24:270:THR:HG23  | 1.87                     | 0.55              |
| 11:A40:212:LYS:NZ  | 11:A40:585:MET:HE1   | 2.10                     | 0.55              |
| 11:A40:362:ARG:CG  | 11:A40:366:ARG:CZ    | 2.85                     | 0.55              |
| 11:A40:437:LEU:CD1 | 11:A40:454:LYS:HZ3   | 2.20                     | 0.55              |
| 10:C:615:GLU:HA    | 10:C:619:LEU:HD12    | 1.88                     | 0.55              |
| 10:C8:643:LEU:CB   | 10:C8:679:ARG:HH12   | 2.20                     | 0.55              |
| 10:C8:1337:LEU:CD2 | 16:A8:126:ARG:HH11   | 2.20                     | 0.55              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A16:20:LEU:HD11  | 21:H:346:THR:CG2     | 2.37                     | 0.55              |
| 11:A32:240:GLU:O    | 11:A32:242:THR:N     | 2.39                     | 0.55              |
| 18:B:720:PHE:CE1    | 18:B:724:LEU:HD11    | 2.42                     | 0.55              |
| 18:B8:1137:ASP:OD1  | 18:B8:1138:PRO:HD2   | 2.06                     | 0.55              |
| 18:B8:1434:VAL:HG13 | 18:B8:1458:LEU:HD22  | 1.87                     | 0.55              |
| 20:E:355:PRO:CA     | 20:E:454:MET:CE      | 2.68                     | 0.55              |
| 19:48:250:ILE:CB    | 20:E8:165:ARG:NH2    | 2.62                     | 0.55              |
| 22:I24:328:TYR:CE1  | 23:J24:717:ILE:HG21  | 2.42                     | 0.55              |
| 22:I16:131:ARG:HE   | 23:J16:557:ARG:HH22  | 1.52                     | 0.55              |
| 10:C32:60:LYS:HG2   | 10:C32:77:ILE:HD11   | 1.87                     | 0.55              |
| 12:A48:467:SER:O    | 12:A48:469:VAL:N     | 2.40                     | 0.55              |
| 12:A48:557:LEU:HD23 | 12:A48:561:ASP:HB3   | 1.85                     | 0.55              |
| 12:A48:823:VAL:HG12 | 12:A48:830:ILE:HD11  | 1.89                     | 0.55              |
| 1:R:1290:ILE:CD1    | 10:C:605:GLU:OE1     | 2.54                     | 0.55              |
| 1:R8:1442:THR:CG2   | 3:N8:13:ILE:HD12     | 2.33                     | 0.55              |
| 1:R8:1466:LYS:HD2   | 6:O8:160:LEU:HD22    | 1.80                     | 0.55              |
| 2:M8:417:ARG:HH12   | 8:L8:398:ALA:HB1     | 1.72                     | 0.55              |
| 2:M8:552:PHE:HZ     | 2:M8:559:PHE:CE2     | 2.17                     | 0.55              |
| 2:M16:202:LYS:HE2   | 2:M16:206:SER:O      | 2.06                     | 0.55              |
| 5:P:401:ARG:HD3     | 5:P:414:VAL:CG2      | 2.30                     | 0.55              |
| 6:O8:179:LYS:O      | 6:O8:180:GLY:O       | 2.25                     | 0.55              |
| 7:Q8:98:MET:HG2     | 7:Q8:112:MET:HG2     | 1.89                     | 0.55              |
| 5:P16:106:ARG:HH22  | 5:P16:462:ARG:HH12   | 1.53                     | 0.55              |
| 7:Q16:236:HIS:CG    | 7:Q16:237:PRO:HD2    | 2.42                     | 0.55              |
| 7:Q16:265:VAL:HG11  | 7:Q16:271:ALA:CB     | 2.37                     | 0.55              |
| 9:K:926:ILE:CD1     | 9:K:937:ILE:HD11     | 2.37                     | 0.55              |
| 9:K:1019:ARG:CB     | 9:K:1059:ARG:NH1     | 2.69                     | 0.55              |
| 9:K:1164:ARG:HE     | 9:K:1230:LEU:HD12    | 1.72                     | 0.55              |
| 9:K8:840:TRP:CZ3    | 9:K8:907:ILE:CG1     | 2.90                     | 0.55              |
| 10:C16:445:MET:HE1  | 10:C16:462:PHE:CZ    | 2.41                     | 0.55              |
| 11:A24:156:MET:HE1  | 11:A24:555:HIS:C     | 2.32                     | 0.55              |
| 10:C24:1612:SER:O   | 10:C24:1616:ILE:HG13 | 2.07                     | 0.55              |
| 12:A:696:ILE:HD11   | 12:A:728:ILE:CD1     | 2.37                     | 0.55              |
| 13:V:753:GLY:O      | 13:V:757:SER:OG      | 2.24                     | 0.55              |
| 13:V:783:TRP:CZ2    | 14:W:671:GLU:CA      | 2.86                     | 0.55              |
| 13:V:816:LYS:O      | 13:V:819:ALA:HB3     | 2.07                     | 0.55              |
| 14:W:518:GLU:H      | 14:W:605:ASN:HD21    | 1.55                     | 0.55              |
| 15:J:658:LEU:HD23   | 15:J:661:MET:CE      | 2.36                     | 0.55              |
| 15:J:678:GLY:O      | 15:J:680:LEU:N       | 2.40                     | 0.55              |
| 10:C:962:PHE:CZ     | 10:C:997:ILE:CD1     | 2.90                     | 0.55              |
| 10:C:1286:MET:HE3   | 10:C:1344:VAL:CG1    | 2.37                     | 0.55              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:1612:SER:O      | 10:C:1616:ILE:HG13   | 2.07                     | 0.55              |
| 10:C8:1614:LEU:CD1   | 10:C8:1635:LEU:HD23  | 2.36                     | 0.55              |
| 11:A16:91:GLU:OE2    | 18:B:1112:LYS:NZ     | 2.40                     | 0.55              |
| 11:A16:122:LYS:NZ    | 18:B:1757:GLU:CD     | 2.65                     | 0.55              |
| 11:A16:362:ARG:HG2   | 11:A16:366:ARG:NH1   | 2.21                     | 0.55              |
| 18:B:488:ASP:HA      | 18:B:554:SER:OG      | 2.07                     | 0.55              |
| 18:B:904:ALA:HB3     | 18:B:917:PHE:HZ      | 1.72                     | 0.55              |
| 18:B:1161:LEU:CD1    | 18:B:1403:ILE:CD1    | 2.76                     | 0.55              |
| 18:B:1841:VAL:HG21   | 18:B:1857:PRO:HG3    | 1.89                     | 0.55              |
| 18:B8:230:ASN:OD1    | 18:B8:233:ARG:HB2    | 2.06                     | 0.55              |
| 18:B8:488:ASP:HA     | 18:B8:554:SER:OG     | 2.07                     | 0.55              |
| 10:C32:18:THR:CG2    | 10:C32:883:GLU:HG2   | 2.36                     | 0.55              |
| 10:C32:275:ALA:CB    | 10:C32:326:LEU:HD12  | 2.37                     | 0.55              |
| 10:C32:879:LEU:HD21  | 10:C32:944:MET:HG3   | 1.89                     | 0.55              |
| 10:C32:906:ARG:HB3   | 10:C32:907:PRO:HD2   | 1.89                     | 0.55              |
| 12:A48:515:LEU:HD21  | 12:A48:565:GLU:OE2   | 2.07                     | 0.55              |
| 2:M:217:ILE:HD11     | 3:N:8:THR:HG21       | 1.87                     | 0.54              |
| 3:N16:116:ILE:CG2    | 3:N16:177:TYR:HE1    | 2.19                     | 0.54              |
| 5:P:193:VAL:HG22     | 5:P:364:VAL:HG13     | 1.89                     | 0.54              |
| 5:P:310:ARG:NH1      | 5:P:372:PRO:HG3      | 2.22                     | 0.54              |
| 7:Q:211:GLY:O        | 7:Q:212:GLU:CG       | 2.54                     | 0.54              |
| 5:P16:510:ILE:HD11   | 7:Q16:183:ARG:NH1    | 2.23                     | 0.54              |
| 6:O16:179:LYS:O      | 6:O16:180:GLY:C      | 2.49                     | 0.54              |
| 7:Q16:258:ARG:C      | 7:Q16:259:TRP:CD1    | 2.86                     | 0.54              |
| 8:L16:621:SER:HB3    | 8:L16:657:TYR:HD1    | 1.69                     | 0.54              |
| 9:K:1249:MET:HA      | 9:K:1254:PHE:CD1     | 2.42                     | 0.54              |
| 9:K8:621:ASN:OD1     | 9:K8:622:VAL:N       | 2.40                     | 0.54              |
| 10:C16:407:LYS:HG3   | 10:C16:465:PHE:HE1   | 1.64                     | 0.54              |
| 10:C16:1465:LEU:HD23 | 11:A24:124:ASN:OD1   | 2.07                     | 0.54              |
| 10:C16:1535:LEU:CB   | 10:C16:1548:ILE:HD13 | 2.37                     | 0.54              |
| 10:C16:1708:ARG:HH11 | 21:H:279:GLU:HB2     | 1.72                     | 0.54              |
| 10:C24:172:ILE:HG23  | 10:C24:240:ILE:HD12  | 1.89                     | 0.54              |
| 10:C24:513:LEU:HD12  | 10:C24:546:LEU:HD23  | 1.90                     | 0.54              |
| 10:C24:667:ILE:CG1   | 10:C24:670:GLU:H     | 2.17                     | 0.54              |
| 12:A:124:ASN:OD1     | 10:C:1465:LEU:HD23   | 2.07                     | 0.54              |
| 12:A:515:LEU:HD21    | 12:A:565:GLU:OE2     | 2.07                     | 0.54              |
| 10:C:1340:PRO:CG     | 10:C:1746:GLY:HA3    | 2.35                     | 0.54              |
| 10:C8:172:ILE:HG23   | 10:C8:240:ILE:HD12   | 1.89                     | 0.54              |
| 10:C8:1593:TRP:N     | 10:C8:1594:PRO:CD    | 2.71                     | 0.54              |
| 11:A16:375:ALA:N     | 11:A16:376:PRO:HD2   | 2.21                     | 0.54              |
| 11:A32:375:ALA:N     | 11:A32:376:PRO:HD2   | 2.21                     | 0.54              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A32:437:LEU:CD1   | 11:A32:454:LYS:HZ3  | 2.18                     | 0.54              |
| 18:B:957:ALA:HA      | 18:B:964:LEU:HD22   | 1.88                     | 0.54              |
| 18:B:1911:LEU:CA     | 18:B:1960:LEU:CD1   | 2.85                     | 0.54              |
| 18:B8:1139:LYS:CB    | 18:B8:1365:ARG:NH1  | 2.70                     | 0.54              |
| 18:B8:1152:ASP:OD1   | 18:B8:1378:LYS:NZ   | 2.37                     | 0.54              |
| 19:4:56:GLU:C        | 19:4:58:GLU:N       | 2.65                     | 0.54              |
| 22:I8:131:ARG:HE     | 23:J8:557:ARG:HH22  | 1.52                     | 0.54              |
| 22:I24:300:LEU:HD11  | 23:J24:689:LEU:CD2  | 2.37                     | 0.54              |
| 24:D:1013:HIS:CE1    | 24:D:1043:TYR:CE1   | 2.94                     | 0.54              |
| 2:M:217:ILE:HD12     | 3:N:8:THR:CG2       | 2.37                     | 0.54              |
| 2:M:307:PHE:HE1      | 2:M:519:TYR:HB3     | 1.72                     | 0.54              |
| 3:N8:218:TRP:CZ3     | 3:N8:229:ILE:HD11   | 2.43                     | 0.54              |
| 1:R16:1449:TRP:CE3   | 2:M16:160:LEU:CD1   | 2.82                     | 0.54              |
| 2:M16:519:TYR:CE2    | 2:M16:520:ILE:HG13  | 2.41                     | 0.54              |
| 3:N16:218:TRP:CZ3    | 3:N16:229:ILE:HD11  | 2.42                     | 0.54              |
| 5:P8:510:ILE:HD11    | 7:Q8:183:ARG:NH1    | 2.23                     | 0.54              |
| 9:K:959:TRP:HB2      | 9:K:988:PHE:HE1     | 1.73                     | 0.54              |
| 9:K8:1249:MET:HA     | 9:K8:1254:PHE:CD1   | 2.42                     | 0.54              |
| 10:C24:386:ASN:HA    | 10:C24:449:GLU:OE1  | 2.07                     | 0.54              |
| 10:C24:390:HIS:CG    | 10:C24:452:LEU:HG   | 2.34                     | 0.54              |
| 10:C24:758:GLN:NE2   | 10:C24:819:GLN:CG   | 2.69                     | 0.54              |
| 10:C24:1076:TYR:O    | 10:C24:1077:ALA:C   | 2.49                     | 0.54              |
| 10:C24:1337:LEU:CD2  | 11:A40:126:ARG:HH11 | 2.20                     | 0.54              |
| 10:C24:1465:LEU:HD23 | 11:A40:124:ASN:OD1  | 2.07                     | 0.54              |
| 11:A40:273:ARG:NE    | 11:A40:479:LEU:HD23 | 2.19                     | 0.54              |
| 10:C8:182:ASP:CB     | 10:C8:183:PRO:CD    | 2.84                     | 0.54              |
| 10:C8:547:VAL:HG21   | 10:C8:587:TYR:HD2   | 1.73                     | 0.54              |
| 10:C8:1271:PHE:HD1   | 10:C8:1273:GLY:H    | 1.54                     | 0.54              |
| 10:C8:1285:VAL:HA    | 10:C8:1735:TYR:CE2  | 2.32                     | 0.54              |
| 11:A32:122:LYS:CD    | 18:B8:1757:GLU:OE1  | 2.55                     | 0.54              |
| 11:A32:386:GLY:O     | 11:A32:459:ARG:CZ   | 2.53                     | 0.54              |
| 11:A32:696:ILE:HD11  | 11:A32:728:ILE:CD1  | 2.37                     | 0.54              |
| 18:B:90:ILE:CD1      | 18:B:105:VAL:HG22   | 2.36                     | 0.54              |
| 23:J24:678:GLY:O     | 23:J24:680:LEU:N    | 2.40                     | 0.54              |
| 21:H16:193:LEU:HD21  | 21:H16:195:GLN:NE2  | 2.15                     | 0.54              |
| 1:R8:1145:LYS:HG2    | 24:D40:1410:GLU:OE1 | 2.07                     | 0.54              |
| 3:N16:221:ASN:C      | 3:N16:223:GLY:H     | 2.16                     | 0.54              |
| 7:Q:298:SER:C        | 7:Q:300:SER:H       | 2.16                     | 0.54              |
| 5:P8:451:LYS:HD3     | 6:O8:312:ASN:O      | 2.08                     | 0.54              |
| 7:Q8:219:GLY:C       | 7:Q8:221:TRP:H      | 2.15                     | 0.54              |
| 7:Q16:125:TYR:HD1    | 7:Q16:167:GLY:HA2   | 1.72                     | 0.54              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 9:K:1019:ARG:HB3     | 9:K:1059:ARG:HH11   | 1.72                     | 0.54              |
| 11:A24:823:VAL:HG12  | 11:A24:830:ILE:HD11 | 1.89                     | 0.54              |
| 10:C24:325:MET:HE2   | 10:C24:352:LEU:HD11 | 1.90                     | 0.54              |
| 10:C24:667:ILE:CG1   | 10:C24:670:GLU:O    | 2.55                     | 0.54              |
| 10:C24:1477:GLN:HG2  | 24:D24:1407:PHE:HB3 | 1.89                     | 0.54              |
| 10:C24:1708:ARG:HH12 | 21:H24:275:LYS:C    | 2.15                     | 0.54              |
| 11:A40:445:ASN:ND2   | 17:F16:65:ARG:HH12  | 1.99                     | 0.54              |
| 11:A40:468:VAL:HG21  | 24:D32:1100:GLN:CB  | 2.37                     | 0.54              |
| 11:A40:524:GLU:OE2   | 11:A40:530:TYR:CD2  | 2.60                     | 0.54              |
| 12:A:362:ARG:CG      | 12:A:366:ARG:CZ     | 2.85                     | 0.54              |
| 12:A:375:ALA:N       | 12:A:376:PRO:HD2    | 2.21                     | 0.54              |
| 10:C:1154:TRP:CE2    | 10:C:1158:HIS:CE1   | 2.94                     | 0.54              |
| 10:C:1801:SER:HB3    | 10:C:1802:PRO:HD3   | 1.90                     | 0.54              |
| 10:C8:643:LEU:HB3    | 10:C8:679:ARG:CZ    | 2.38                     | 0.54              |
| 10:C8:1121:ILE:HG23  | 10:C8:1133:ILE:HD11 | 1.89                     | 0.54              |
| 10:C8:1286:MET:HE3   | 10:C8:1344:VAL:CG1  | 2.37                     | 0.54              |
| 10:C8:1286:MET:CE    | 10:C8:1344:VAL:CG1  | 2.84                     | 0.54              |
| 10:C8:1682:VAL:HG22  | 10:C8:1758:LEU:CD2  | 2.36                     | 0.54              |
| 11:A16:707:LEU:HB2   | 24:D16:1398:ARG:CZ  | 2.29                     | 0.54              |
| 18:B:1139:LYS:CB     | 18:B:1365:ARG:NH1   | 2.70                     | 0.54              |
| 18:B8:409:LEU:O      | 18:B8:462:ARG:NH1   | 2.37                     | 0.54              |
| 18:B8:1700:LEU:CD2   | 18:B8:1833:PHE:CD2  | 2.89                     | 0.54              |
| 18:B8:1841:VAL:HG21  | 18:B8:1857:PRO:HG3  | 1.89                     | 0.54              |
| 20:E:350:GLU:C       | 20:E:352:PHE:N      | 2.64                     | 0.54              |
| 21:H8:179:GLU:O      | 21:H8:186:ARG:NH2   | 2.40                     | 0.54              |
| 22:I8:300:LEU:HD11   | 23:J8:689:LEU:CD2   | 2.37                     | 0.54              |
| 10:C32:325:MET:HE2   | 10:C32:352:LEU:HD11 | 1.89                     | 0.54              |
| 10:C32:1286:MET:HE3  | 10:C32:1344:VAL:CG1 | 2.37                     | 0.54              |
| 10:C32:1637:PHE:CD1  | 12:A48:136:LEU:HD11 | 2.41                     | 0.54              |
| 1:R:1334:GLU:HB3     | 10:C:1170:VAL:HG22  | 1.88                     | 0.54              |
| 2:M8:339:GLU:C       | 2:M8:341:ASP:H      | 2.16                     | 0.54              |
| 2:M8:844:VAL:HG13    | 4:T8:660:LEU:HD11   | 1.89                     | 0.54              |
| 2:M16:507:LEU:CD2    | 2:M16:514:TRP:CE3   | 2.90                     | 0.54              |
| 2:M16:614:TYR:CZ     | 2:M16:618:HIS:CE1   | 2.95                     | 0.54              |
| 2:M16:832:PRO:HB2    | 2:M16:834:ASP:OD1   | 2.08                     | 0.54              |
| 6:O:179:LYS:O        | 6:O:180:GLY:C       | 2.49                     | 0.54              |
| 5:P8:233:TYR:CE1     | 5:P8:237:MET:CE     | 2.90                     | 0.54              |
| 5:P8:614:VAL:H       | 5:P8:629:ARG:CZ     | 2.18                     | 0.54              |
| 5:P8:624:HIS:HE1     | 5:P8:660:ARG:NH2    | 2.06                     | 0.54              |
| 5:P16:188:LEU:HD23   | 5:P16:380:MET:CE    | 2.35                     | 0.54              |
| 5:P16:347:GLY:O      | 5:P16:370:LEU:HD21  | 2.08                     | 0.54              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 5:P16:675:LEU:HD12  | 5:P16:704:LEU:CD1    | 2.36                     | 0.54              |
| 6:O16:133:LEU:HD22  | 6:O16:189:LEU:HD22   | 1.87                     | 0.54              |
| 9:K:1065:GLU:C      | 9:K:1067:VAL:N       | 2.64                     | 0.54              |
| 9:K8:926:ILE:CD1    | 9:K8:937:ILE:HD11    | 2.37                     | 0.54              |
| 10:C16:325:MET:HE2  | 10:C16:352:LEU:HD11  | 1.90                     | 0.54              |
| 10:C16:1612:SER:O   | 10:C16:1616:ILE:HG13 | 2.07                     | 0.54              |
| 11:A24:20:LEU:HD11  | 21:H8:346:THR:CG2    | 2.37                     | 0.54              |
| 10:C24:394:SER:OG   | 10:C24:452:LEU:CD1   | 2.49                     | 0.54              |
| 10:C24:1286:MET:HE3 | 10:C24:1344:VAL:CG1  | 2.37                     | 0.54              |
| 11:A40:323:LEU:CD2  | 17:F16:74:ILE:HD12   | 2.36                     | 0.54              |
| 11:A40:362:ARG:HG2  | 11:A40:366:ARG:NH1   | 2.21                     | 0.54              |
| 10:C:182:ASP:CB     | 10:C:183:PRO:CD      | 2.84                     | 0.54              |
| 10:C:699:HIS:O      | 10:C:703:SER:OG      | 2.24                     | 0.54              |
| 10:C:1002:LEU:CD1   | 10:C:1019:ARG:NH1    | 2.64                     | 0.54              |
| 10:C:1121:ILE:HG23  | 10:C:1133:ILE:HD11   | 1.89                     | 0.54              |
| 10:C8:325:MET:HE2   | 10:C8:352:LEU:HD11   | 1.90                     | 0.54              |
| 10:C8:906:ARG:HB3   | 10:C8:907:PRO:HD2    | 1.90                     | 0.54              |
| 10:C8:1535:LEU:CB   | 10:C8:1548:ILE:HD13  | 2.37                     | 0.54              |
| 11:A16:707:LEU:CD1  | 11:A16:767:ARG:HH22  | 2.17                     | 0.54              |
| 11:A16:806:GLN:CG   | 11:A16:847:ARG:HH22  | 2.16                     | 0.54              |
| 11:A32:707:LEU:CD1  | 11:A32:767:ARG:HH22  | 2.17                     | 0.54              |
| 18:B:409:LEU:O      | 18:B:462:ARG:NH1     | 2.37                     | 0.54              |
| 18:B:1102:LYS:NZ    | 18:B:1354:ASP:CG     | 2.59                     | 0.54              |
| 18:B8:241:TYR:HB2   | 18:B8:271:LEU:CD2    | 2.32                     | 0.54              |
| 18:B8:268:GLN:HE22  | 18:B8:323:GLU:HB3    | 1.69                     | 0.54              |
| 18:B8:904:ALA:HB3   | 18:B8:917:PHE:HZ     | 1.72                     | 0.54              |
| 19:4:250:ILE:HG23   | 20:E:165:ARG:CZ      | 2.36                     | 0.54              |
| 20:E:130:GLY:N      | 20:E:131:PRO:CD      | 2.70                     | 0.54              |
| 20:E8:355:PRO:C     | 20:E8:454:MET:HE1    | 2.32                     | 0.54              |
| 21:H:179:GLU:O      | 21:H:186:ARG:NH2     | 2.40                     | 0.54              |
| 21:H:312:GLN:NE2    | 21:H:316:ILE:HD11    | 2.21                     | 0.54              |
| 23:J32:718:GLN:CD   | 23:J32:737:TRP:CH2   | 2.83                     | 0.54              |
| 21:H8:312:GLN:NE2   | 21:H8:316:ILE:HD11   | 2.21                     | 0.54              |
| 21:H8:322:LEU:HD22  | 22:I8:300:LEU:HG     | 1.89                     | 0.54              |
| 21:H16:253:ARG:NE   | 23:J16:621:GLU:OE2   | 2.38                     | 0.54              |
| 22:I16:368:VAL:CG2  | 23:J16:591:LYS:NZ    | 2.71                     | 0.54              |
| 10:C32:1337:LEU:CD2 | 12:A48:126:ARG:HH11  | 2.20                     | 0.54              |
| 10:C32:1535:LEU:CB  | 10:C32:1548:ILE:HD13 | 2.37                     | 0.54              |
| 10:C32:1612:SER:O   | 10:C32:1616:ILE:HG13 | 2.07                     | 0.54              |
| 12:A48:782:PRO:C    | 12:A48:783:PHE:CD2   | 2.86                     | 0.54              |
| 2:M:810:LEU:HD23    | 2:M:819:GLN:HG2      | 1.89                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:R8:1347:HIS:CE1   | 1:R8:1349:ARG:HB2   | 2.43                     | 0.54              |
| 1:R16:1139:ARG:HB2  | 1:R16:1157:ARG:NH2  | 2.22                     | 0.54              |
| 2:M16:847:PHE:CD1   | 4:T16:656:TRP:HE3   | 2.21                     | 0.54              |
| 5:P:624:HIS:CE1     | 5:P:660:ARG:NH2     | 2.76                     | 0.54              |
| 7:Q:219:GLY:C       | 7:Q:221:TRP:H       | 2.15                     | 0.54              |
| 5:P8:347:GLY:O      | 5:P8:370:LEU:HD21   | 2.08                     | 0.54              |
| 7:Q8:265:VAL:HG11   | 7:Q8:271:ALA:HB1    | 1.89                     | 0.54              |
| 5:P16:607:PHE:CB    | 5:P16:629:ARG:CZ    | 2.85                     | 0.54              |
| 5:P16:634:MET:HG3   | 5:P16:671:MET:SD    | 2.47                     | 0.54              |
| 7:Q16:298:SER:C     | 7:Q16:300:SER:H     | 2.16                     | 0.54              |
| 8:L8:614:GLU:OE1    | 8:L8:649:LYS:NZ     | 2.40                     | 0.54              |
| 9:K:959:TRP:NE1     | 9:K:992:GLN:OE1     | 2.40                     | 0.54              |
| 9:K8:923:ILE:HG21   | 9:K8:929:ARG:HH21   | 1.72                     | 0.54              |
| 9:K8:1085:TYR:HE1   | 9:K8:1093:SER:O     | 1.86                     | 0.54              |
| 10:C16:513:LEU:HD12 | 10:C16:546:LEU:HD23 | 1.90                     | 0.54              |
| 10:C16:879:LEU:HD21 | 10:C16:944:MET:HG3  | 1.90                     | 0.54              |
| 10:C16:906:ARG:HB3  | 10:C16:907:PRO:HD2  | 1.90                     | 0.54              |
| 11:A24:362:ARG:HG2  | 11:A24:366:ARG:NH1  | 2.21                     | 0.54              |
| 10:C24:653:TYR:N    | 10:C24:654:PRO:HD3  | 2.22                     | 0.54              |
| 12:A:587:VAL:CG2    | 12:A:636:PHE:HE1    | 2.18                     | 0.54              |
| 10:C:325:MET:HE2    | 10:C:352:LEU:HD11   | 1.89                     | 0.54              |
| 10:C:667:ILE:CG1    | 10:C:670:GLU:O      | 2.55                     | 0.54              |
| 10:C8:1109:VAL:HG12 | 10:C8:1109:VAL:O    | 2.07                     | 0.54              |
| 10:C8:1335:ILE:O    | 10:C8:1336:ALA:C    | 2.48                     | 0.54              |
| 11:A16:240:GLU:O    | 11:A16:242:THR:N    | 2.40                     | 0.54              |
| 18:B:1505:MET:CE    | 18:B:1518:VAL:CG2   | 2.84                     | 0.54              |
| 18:B:1579:ASN:HD21  | 24:D16:1403:LEU:CD2 | 2.20                     | 0.54              |
| 18:B8:1911:LEU:CA   | 18:B8:1960:LEU:HD11 | 2.37                     | 0.54              |
| 21:H:253:ARG:NE     | 23:J32:621:GLU:OE2  | 2.38                     | 0.54              |
| 23:J24:718:GLN:CD   | 23:J24:737:TRP:CH2  | 2.83                     | 0.54              |
| 10:C32:653:TYR:N    | 10:C32:654:PRO:HD3  | 2.22                     | 0.54              |
| 10:C32:1378:LYS:HA  | 10:C32:1381:ALA:HB2 | 1.89                     | 0.54              |
| 1:R:979:GLN:OE1     | 24:D:1438:ALA:HB2   | 2.07                     | 0.54              |
| 1:R:1022:TYR:CE1    | 24:D:1441:PRO:CG    | 2.86                     | 0.54              |
| 1:R8:1139:ARG:HH11  | 1:R8:1157:ARG:CZ    | 2.02                     | 0.54              |
| 1:R8:1204:ASN:C     | 1:R8:1206:GLN:N     | 2.66                     | 0.54              |
| 2:M16:307:PHE:HE1   | 2:M16:519:TYR:HB3   | 1.72                     | 0.54              |
| 5:P:451:LYS:HD3     | 6:O:312:ASN:O       | 2.08                     | 0.54              |
| 5:P:510:ILE:HD11    | 7:Q:183:ARG:NH1     | 2.23                     | 0.54              |
| 5:P8:615:HIS:H      | 5:P8:629:ARG:NH1    | 2.03                     | 0.54              |
| 5:P16:214:LEU:HD23  | 5:P16:236:VAL:HG13  | 1.81                     | 0.54              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K8:950:LYS:HE3     | 9:K8:977:GLU:CB      | 2.37                     | 0.54              |
| 10:C16:275:ALA:CB    | 10:C16:326:LEU:HD12  | 2.37                     | 0.54              |
| 10:C16:626:GLN:O     | 10:C16:627:VAL:C     | 2.38                     | 0.54              |
| 10:C16:879:LEU:HD21  | 10:C16:944:MET:CG    | 2.38                     | 0.54              |
| 10:C16:1009:GLN:C    | 10:C16:1192:ARG:NH2  | 2.60                     | 0.54              |
| 10:C16:1682:VAL:HG22 | 10:C16:1758:LEU:CD2  | 2.36                     | 0.54              |
| 10:C24:668:ALA:O     | 10:C24:704:MET:HE1   | 2.08                     | 0.54              |
| 12:A:512:VAL:HG12    | 12:A:512:VAL:O       | 2.08                     | 0.54              |
| 12:A:823:VAL:HG12    | 12:A:830:ILE:HD11    | 1.89                     | 0.54              |
| 14:W:586:ILE:HD12    | 15:J:569:ALA:O       | 2.07                     | 0.54              |
| 14:W:598:ILE:HD13    | 14:W:626:LEU:HB3     | 1.89                     | 0.54              |
| 10:C8:1340:PRO:HG2   | 10:C8:1746:GLY:CA    | 2.34                     | 0.54              |
| 11:A16:512:VAL:O     | 11:A16:512:VAL:HG12  | 2.08                     | 0.54              |
| 11:A32:20:LEU:HD11   | 21:H24:346:THR:CG2   | 2.37                     | 0.54              |
| 11:A32:515:LEU:HD21  | 11:A32:565:GLU:OE2   | 2.07                     | 0.54              |
| 11:A32:542:VAL:HG11  | 11:A32:596:THR:HG23  | 1.90                     | 0.54              |
| 18:B:582:LEU:O       | 18:B:586:VAL:HG22    | 2.07                     | 0.54              |
| 18:B8:191:PHE:CE2    | 18:B8:192:PRO:O      | 2.60                     | 0.54              |
| 18:B8:345:GLU:HA     | 18:B8:351:MET:CE     | 2.35                     | 0.54              |
| 18:B8:582:LEU:O      | 18:B8:586:VAL:HG22   | 2.07                     | 0.54              |
| 20:E:429:PRO:HG2     | 24:D:69:VAL:CB       | 2.38                     | 0.54              |
| 20:E8:350:GLU:C      | 20:E8:352:PHE:H      | 2.15                     | 0.54              |
| 20:E8:448:LYS:HB2    | 20:E8:451:ILE:HD12   | 1.88                     | 0.54              |
| 22:I:300:LEU:HD11    | 23:J32:689:LEU:CD2   | 2.38                     | 0.54              |
| 22:I8:332:MET:SD     | 23:J8:732:MET:HE1    | 2.48                     | 0.54              |
| 23:J8:734:PRO:O      | 23:J8:735:LYS:C      | 2.46                     | 0.54              |
| 24:D8:853:MET:HB3    | 24:D8:885:TYR:CD2    | 2.42                     | 0.54              |
| 24:D8:1452:LYS:NZ    | 24:D16:971:HIS:NE2   | 2.42                     | 0.54              |
| 24:D32:1284:ILE:CD1  | 24:D32:1329:VAL:HG21 | 2.38                     | 0.54              |
| 24:D40:749:ARG:CZ    | 24:D40:964:LEU:HA    | 2.37                     | 0.54              |
| 10:C32:8:VAL:HG23    | 10:C32:133:THR:HG1   | 1.73                     | 0.54              |
| 10:C32:1251:PHE:HZ   | 10:C32:1319:ARG:HH12 | 1.39                     | 0.54              |
| 10:C32:1335:ILE:O    | 10:C32:1336:ALA:C    | 2.48                     | 0.54              |
| 10:C32:1465:LEU:HD23 | 12:A48:124:ASN:OD1   | 2.07                     | 0.54              |
| 2:M8:166:THR:N       | 2:M8:169:THR:OG1     | 2.33                     | 0.54              |
| 2:M8:251:HIS:NE2     | 2:M8:273:VAL:HG21    | 2.23                     | 0.54              |
| 2:M16:166:THR:N      | 2:M16:169:THR:OG1    | 2.33                     | 0.54              |
| 5:P:401:ARG:NE       | 5:P:414:VAL:HG21     | 2.18                     | 0.54              |
| 5:P8:310:ARG:NH1     | 5:P8:372:PRO:HG3     | 2.22                     | 0.54              |
| 6:O8:130:ASP:O       | 6:O8:166:PRO:HG2     | 2.07                     | 0.54              |
| 7:Q8:258:ARG:C       | 7:Q8:259:TRP:CD1     | 2.86                     | 0.54              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:O16:130:ASP:O      | 6:O16:166:PRO:HG2    | 2.07                     | 0.54              |
| 9:K:840:TRP:CZ3      | 9:K:907:ILE:CG1      | 2.90                     | 0.54              |
| 9:K:1230:LEU:HD23    | 9:K:1244:VAL:HG23    | 1.88                     | 0.54              |
| 11:A24:86:LEU:HD23   | 22:I8:301:LEU:HD23   | 1.90                     | 0.54              |
| 11:A24:234:TYR:CZ    | 11:A24:249:MET:HB3   | 2.43                     | 0.54              |
| 10:C24:1535:LEU:CB   | 10:C24:1548:ILE:HD13 | 2.37                     | 0.54              |
| 11:A40:515:LEU:HD21  | 11:A40:565:GLU:OE2   | 2.07                     | 0.54              |
| 12:A:524:GLU:OE2     | 12:A:530:TYR:CD2     | 2.60                     | 0.54              |
| 12:A:560:MET:HE2     | 12:A:615:GLN:NE2     | 1.97                     | 0.54              |
| 13:V:776:LEU:CD1     | 14:W:664:ASN:OD1     | 2.55                     | 0.54              |
| 14:W:714:LEU:C       | 10:C8:1568:ARG:CZ    | 2.80                     | 0.54              |
| 10:C:879:LEU:HD21    | 10:C:944:MET:HG3     | 1.89                     | 0.54              |
| 10:C:1593:TRP:N      | 10:C:1594:PRO:CD     | 2.71                     | 0.54              |
| 10:C:1796:LEU:HG     | 10:C:1800:LEU:HD12   | 1.88                     | 0.54              |
| 11:A16:362:ARG:CG    | 11:A16:366:ARG:CZ    | 2.85                     | 0.54              |
| 11:A16:524:GLU:OE2   | 11:A16:530:TYR:CD2   | 2.60                     | 0.54              |
| 11:A16:696:ILE:HD11  | 11:A16:728:ILE:CD1   | 2.37                     | 0.54              |
| 11:A32:512:VAL:HG12  | 11:A32:512:VAL:O     | 2.08                     | 0.54              |
| 18:B:761:TRP:HE1     | 18:B:826:GLU:CD      | 2.16                     | 0.54              |
| 18:B:1528:PRO:HA     | 18:B:1531:TRP:CD1    | 2.42                     | 0.54              |
| 18:B8:52:SER:CB      | 18:B8:178:ARG:HH21   | 2.21                     | 0.54              |
| 18:B8:94:LEU:CD2     | 18:B8:132:LEU:CD2    | 2.77                     | 0.54              |
| 18:B8:720:PHE:CE1    | 18:B8:724:LEU:HD11   | 2.42                     | 0.54              |
| 19:4:100:ILE:CG2     | 19:4:102:LEU:CG      | 2.74                     | 0.54              |
| 20:E8:130:GLY:N      | 20:E8:131:PRO:CD     | 2.70                     | 0.54              |
| 24:D24:1170:VAL:HG22 | 24:D24:1232:VAL:CG2  | 2.38                     | 0.54              |
| 24:D32:1109:LEU:CD2  | 24:D32:1156:SER:CB   | 2.82                     | 0.54              |
| 10:C32:547:VAL:HG21  | 10:C32:587:TYR:HD2   | 1.73                     | 0.54              |
| 10:C32:663:ILE:CG2   | 10:C32:667:ILE:HG23  | 2.38                     | 0.54              |
| 3:N8:221:ASN:C       | 3:N8:223:GLY:H       | 2.16                     | 0.54              |
| 1:R16:1379:GLN:NE2   | 1:R16:1416:TYR:CE1   | 2.75                     | 0.54              |
| 5:P:12:GLU:HB2       | 5:P:78:GLY:HA3       | 1.88                     | 0.54              |
| 5:P8:43:TRP:HH2      | 5:P8:76:LEU:CD1      | 2.21                     | 0.54              |
| 9:K:1146:ILE:HD13    | 9:K:1208:GLN:OE1     | 2.05                     | 0.54              |
| 9:K8:919:MET:SD      | 9:K8:919:MET:C       | 2.91                     | 0.54              |
| 9:K8:1039:ASP:O      | 9:K8:1043:THR:OG1    | 2.26                     | 0.54              |
| 10:C16:1593:TRP:N    | 10:C16:1594:PRO:CD   | 2.71                     | 0.54              |
| 11:A24:515:LEU:HD21  | 11:A24:565:GLU:OE2   | 2.07                     | 0.54              |
| 10:C24:761:VAL:CG2   | 10:C24:826:TYR:HA    | 2.35                     | 0.54              |
| 10:C24:1724:VAL:HG22 | 10:C24:1736:ILE:CD1  | 2.38                     | 0.54              |
| 14:W:514:THR:N       | 14:W:607:ARG:NH1     | 2.40                     | 0.54              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C8:1682:VAL:HG22  | 10:C8:1758:LEU:HD23 | 1.89                     | 0.54              |
| 11:A16:467:SER:O     | 11:A16:469:VAL:N    | 2.40                     | 0.54              |
| 11:A16:542:VAL:HG11  | 11:A16:596:THR:HG23 | 1.90                     | 0.54              |
| 11:A32:124:ASN:HB2   | 18:B8:1523:ARG:NH1  | 2.22                     | 0.54              |
| 11:A32:362:ARG:CG    | 11:A32:366:ARG:CZ   | 2.85                     | 0.54              |
| 11:A32:686:VAL:O     | 11:A32:686:VAL:HG12 | 2.08                     | 0.54              |
| 18:B:135:TYR:CZ      | 18:B:139:ARG:HD2    | 2.43                     | 0.54              |
| 18:B8:684:ILE:HD11   | 24:D32:1065:ALA:CB  | 2.38                     | 0.54              |
| 18:B8:783:LYS:HE3    | 24:D32:1064:GLY:CA  | 2.23                     | 0.54              |
| 19:4:360:TRP:HD1     | 19:4:366:ARG:O      | 1.91                     | 0.54              |
| 20:E:25:PRO:HG3      | 20:E:237:ILE:CD1    | 2.37                     | 0.54              |
| 20:E:344:PRO:C       | 24:D:121:GLU:OE1    | 2.49                     | 0.54              |
| 19:48:250:ILE:HG23   | 20:E8:165:ARG:CZ    | 2.36                     | 0.54              |
| 20:E8:50:PHE:CZ      | 20:E8:54:HIS:NE2    | 2.76                     | 0.54              |
| 23:J8:682:ALA:C      | 23:J8:684:ASP:H     | 2.15                     | 0.54              |
| 22:I16:300:LEU:HD11  | 23:J16:689:LEU:CD2  | 2.37                     | 0.54              |
| 10:C32:325:MET:HE1   | 10:C32:352:LEU:HD21 | 1.90                     | 0.54              |
| 10:C32:758:GLN:NE2   | 10:C32:819:GLN:CG   | 2.69                     | 0.54              |
| 12:A48:362:ARG:CG    | 12:A48:366:ARG:CZ   | 2.85                     | 0.54              |
| 12:A48:696:ILE:HD11  | 12:A48:728:ILE:CD1  | 2.38                     | 0.54              |
| 1:R:1473:HIS:HD2     | 6:O:160:LEU:HB3     | 1.72                     | 0.54              |
| 1:R8:1349:ARG:CG     | 1:R8:1390:GLU:HB3   | 2.38                     | 0.54              |
| 2:M8:307:PHE:HE1     | 2:M8:519:TYR:HB3    | 1.73                     | 0.54              |
| 2:M8:519:TYR:CE2     | 2:M8:520:ILE:HG13   | 2.42                     | 0.54              |
| 4:T16:671:ILE:CD1    | 5:P16:698:GLY:HA3   | 2.37                     | 0.54              |
| 5:P:16:PHE:CE1       | 6:O:311:LEU:CG      | 2.91                     | 0.54              |
| 5:P:486:CYS:HB2      | 5:P:490:GLY:HA3     | 1.90                     | 0.54              |
| 5:P:600:PHE:CE1      | 5:P:638:SER:HB2     | 2.43                     | 0.54              |
| 7:Q:258:ARG:C        | 7:Q:259:TRP:CD1     | 2.86                     | 0.54              |
| 7:Q:297:VAL:HG21     | 7:Q:318:GLU:OE1     | 2.08                     | 0.54              |
| 5:P8:106:ARG:HH22    | 5:P8:462:ARG:HH12   | 1.53                     | 0.54              |
| 5:P16:16:PHE:CE1     | 6:O16:311:LEU:CG    | 2.91                     | 0.54              |
| 9:K:1056:VAL:CG2     | 9:K:1059:ARG:HH21   | 2.19                     | 0.54              |
| 9:K:1259:LYS:O       | 9:K:1263:THR:OG1    | 2.20                     | 0.54              |
| 9:K8:1176:ASP:OD1    | 9:K8:1251:HIS:NE2   | 2.40                     | 0.54              |
| 10:C16:667:ILE:CG1   | 10:C16:670:GLU:O    | 2.55                     | 0.54              |
| 10:C16:1801:SER:HB3  | 10:C16:1802:PRO:HD3 | 1.90                     | 0.54              |
| 10:C24:1109:VAL:HG12 | 10:C24:1109:VAL:O   | 2.07                     | 0.54              |
| 12:A:798:PHE:HE2     | 12:A:809:VAL:HG21   | 1.73                     | 0.54              |
| 10:C:297:GLN:OE1     | 10:C:320:TRP:NE1    | 2.37                     | 0.54              |
| 10:C:643:LEU:CD1     | 10:C:679:ARG:HH12   | 2.03                     | 0.54              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:668:ALA:O       | 10:C:704:MET:HE1     | 2.08                     | 0.54              |
| 10:C:906:ARG:HB3     | 10:C:907:PRO:HD2     | 1.90                     | 0.54              |
| 10:C8:1378:LYS:HA    | 10:C8:1381:ALA:HB2   | 1.89                     | 0.54              |
| 11:A32:782:PRO:C     | 11:A32:783:PHE:CD2   | 2.86                     | 0.54              |
| 18:B:187:LEU:HD22    | 18:B:251:PHE:HE2     | 1.71                     | 0.54              |
| 18:B8:1958:ALA:HB2   | 18:B8:1965:LEU:CD1   | 2.37                     | 0.54              |
| 20:E:350:GLU:C       | 20:E:352:PHE:H       | 2.15                     | 0.54              |
| 19:48:15:ILE:HD12    | 19:48:20:ILE:CD1     | 2.38                     | 0.54              |
| 19:48:360:TRP:HD1    | 19:48:366:ARG:O      | 1.91                     | 0.54              |
| 22:I24:131:ARG:CG    | 23:J24:557:ARG:HH22  | 2.11                     | 0.54              |
| 22:I24:332:MET:SD    | 23:J24:732:MET:HE1   | 2.48                     | 0.54              |
| 24:D:1170:VAL:HG22   | 24:D:1232:VAL:CG2    | 2.38                     | 0.54              |
| 24:D40:1170:VAL:HG22 | 24:D40:1232:VAL:CG2  | 2.38                     | 0.54              |
| 10:C32:1593:TRP:N    | 10:C32:1594:PRO:CD   | 2.71                     | 0.54              |
| 10:C32:1724:VAL:HG22 | 10:C32:1736:ILE:CD1  | 2.38                     | 0.54              |
| 12:A48:542:VAL:HG11  | 12:A48:596:THR:HG23  | 1.90                     | 0.54              |
| 1:R:1442:THR:CG2     | 3:N:13:ILE:HD12      | 2.33                     | 0.54              |
| 2:M:503:TYR:CE1      | 2:M:507:LEU:HD11     | 2.43                     | 0.54              |
| 2:M:832:PRO:HB2      | 2:M:834:ASP:OD1      | 2.08                     | 0.54              |
| 1:R8:982:GLU:HG3     | 24:D40:1436:ARG:CZ   | 2.38                     | 0.54              |
| 2:M8:810:LEU:HD23    | 2:M8:819:GLN:HG2     | 1.89                     | 0.54              |
| 1:R16:1204:ASN:C     | 1:R16:1206:GLN:N     | 2.66                     | 0.54              |
| 2:M16:191:TRP:CH2    | 2:M16:222:ILE:HD11   | 2.43                     | 0.54              |
| 2:M16:810:LEU:HD23   | 2:M16:819:GLN:HG2    | 1.89                     | 0.54              |
| 5:P:288:ARG:O        | 5:P:299:CYS:HB3      | 2.08                     | 0.54              |
| 6:O:120:LYS:HE3      | 10:C:1163:LEU:HD13   | 1.90                     | 0.54              |
| 6:O8:125:VAL:HG23    | 6:O8:175:TRP:CZ2     | 2.43                     | 0.54              |
| 7:Q8:125:TYR:HD1     | 7:Q8:167:GLY:HA2     | 1.72                     | 0.54              |
| 7:Q8:298:SER:C       | 7:Q8:300:SER:H       | 2.16                     | 0.54              |
| 6:O16:125:VAL:HG23   | 6:O16:175:TRP:CZ2    | 2.43                     | 0.54              |
| 9:K:828:PRO:CB       | 9:K:830:HIS:CE1      | 2.89                     | 0.54              |
| 9:K:879:CYS:CB       | 9:K:900:TYR:CE2      | 2.91                     | 0.54              |
| 9:K:1039:ASP:O       | 9:K:1043:THR:OG1     | 2.26                     | 0.54              |
| 9:K8:975:MET:CE      | 9:K8:989:VAL:CG1     | 2.73                     | 0.54              |
| 9:K8:1133:ILE:HG21   | 9:K8:1166:LEU:HD23   | 1.88                     | 0.54              |
| 9:K16:894:LYS:CE     | 9:K16:1058:GLU:HG3   | 2.38                     | 0.54              |
| 10:C16:699:HIS:O     | 10:C16:703:SER:OG    | 2.23                     | 0.54              |
| 10:C16:1076:TYR:O    | 10:C16:1077:ALA:C    | 2.49                     | 0.54              |
| 10:C16:1251:PHE:HZ   | 10:C16:1319:ARG:HH12 | 1.39                     | 0.54              |
| 10:C16:1642:TYR:CE1  | 10:C16:1646:LEU:HD11 | 2.43                     | 0.54              |
| 11:A24:524:GLU:OE2   | 11:A24:530:TYR:CD2   | 2.60                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C24:547:VAL:HG21 | 10:C24:587:TYR:HD2  | 1.72                     | 0.54              |
| 10:C24:1593:TRP:N   | 10:C24:1594:PRO:CD  | 2.71                     | 0.54              |
| 11:A40:20:LEU:HD11  | 21:H16:346:THR:CG2  | 2.37                     | 0.54              |
| 11:A40:823:VAL:HG12 | 11:A40:830:ILE:HD11 | 1.89                     | 0.54              |
| 12:A:467:SER:O      | 12:A:469:VAL:N      | 2.40                     | 0.54              |
| 12:A:782:PRO:C      | 12:A:783:PHE:CD2    | 2.86                     | 0.54              |
| 13:V:844:MET:C      | 10:C8:1502:ARG:HH22 | 2.16                     | 0.54              |
| 14:W:711:ARG:HD3    | 10:C8:1609:ASP:HB3  | 1.89                     | 0.54              |
| 10:C:325:MET:HE1    | 10:C:352:LEU:HD21   | 1.90                     | 0.54              |
| 10:C8:325:MET:HE1   | 10:C8:352:LEU:HD21  | 1.90                     | 0.54              |
| 10:C8:879:LEU:HD21  | 10:C8:944:MET:CG    | 2.38                     | 0.54              |
| 10:C8:1801:SER:HB3  | 10:C8:1802:PRO:HD3  | 1.90                     | 0.54              |
| 11:A16:91:GLU:OE2   | 18:B:1112:LYS:CE    | 2.55                     | 0.54              |
| 11:A16:798:PHE:HE2  | 11:A16:809:VAL:HG21 | 1.73                     | 0.54              |
| 11:A32:234:TYR:CZ   | 11:A32:249:MET:HB3  | 2.43                     | 0.54              |
| 11:A32:273:ARG:NE   | 11:A32:479:LEU:HD23 | 2.19                     | 0.54              |
| 11:A32:322:ARG:HH11 | 11:A32:351:PHE:HZ   | 1.56                     | 0.54              |
| 18:B:52:SER:CB      | 18:B:178:ARG:HH21   | 2.21                     | 0.54              |
| 18:B:370:TYR:CE1    | 18:B:374:ILE:HD11   | 2.43                     | 0.54              |
| 18:B:856:LEU:CD2    | 18:B:860:HIS:HB3    | 2.37                     | 0.54              |
| 18:B:1958:ALA:HB2   | 18:B:1965:LEU:CD1   | 2.37                     | 0.54              |
| 18:B8:761:TRP:HE1   | 18:B8:826:GLU:CD    | 2.16                     | 0.54              |
| 18:B8:1911:LEU:CB   | 18:B8:1960:LEU:CD1  | 2.86                     | 0.54              |
| 19:48:251:ARG:NH2   | 19:48:254:LEU:HD23  | 2.21                     | 0.54              |
| 21:H:193:LEU:HD21   | 21:H:195:GLN:NE2    | 2.15                     | 0.54              |
| 22:I:332:MET:SD     | 23:J32:732:MET:HE1  | 2.48                     | 0.54              |
| 10:C32:172:ILE:HG23 | 10:C32:240:ILE:HD12 | 1.89                     | 0.54              |
| 10:C32:1801:SER:HB3 | 10:C32:1802:PRO:HD3 | 1.90                     | 0.54              |
| 12:A48:798:PHE:HE2  | 12:A48:809:VAL:HG21 | 1.73                     | 0.54              |
| 2:M:339:GLU:C       | 2:M:341:ASP:H       | 2.16                     | 0.53              |
| 2:M8:847:PHE:CE1    | 4:T8:656:TRP:HB3    | 1.98                     | 0.53              |
| 2:M16:251:HIS:NE2   | 2:M16:273:VAL:HG21  | 2.23                     | 0.53              |
| 5:P8:188:LEU:HD23   | 5:P8:380:MET:CE     | 2.35                     | 0.53              |
| 5:P8:486:CYS:HB2    | 5:P8:490:GLY:HA3    | 1.90                     | 0.53              |
| 7:Q8:265:VAL:HG11   | 7:Q8:271:ALA:CB     | 2.38                     | 0.53              |
| 5:P16:14:VAL:HG22   | 5:P16:419:SER:OG    | 2.07                     | 0.53              |
| 5:P16:165:PRO:O     | 5:P16:202:LEU:HD21  | 2.08                     | 0.53              |
| 5:P16:288:ARG:O     | 5:P16:299:CYS:HB3   | 2.08                     | 0.53              |
| 6:O16:119:ARG:NH2   | 6:O16:182:GLU:CA    | 2.57                     | 0.53              |
| 7:Q16:147:GLU:OE1   | 7:Q16:159:VAL:CG1   | 2.56                     | 0.53              |
| 9:K8:1164:ARG:HE    | 9:K8:1230:LEU:HD12  | 1.72                     | 0.53              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:925:GLU:OE1   | 10:C16:973:LEU:HD23  | 2.08                     | 0.53              |
| 11:A24:273:ARG:NE    | 11:A24:479:LEU:HD23  | 2.19                     | 0.53              |
| 10:C24:854:LEU:CD2   | 10:C24:911:ILE:HD11  | 2.33                     | 0.53              |
| 12:A:126:ARG:HH11    | 10:C:1337:LEU:CD2    | 2.20                     | 0.53              |
| 12:A:542:VAL:HG11    | 12:A:596:THR:HG23    | 1.90                     | 0.53              |
| 14:W:554:LYS:CD      | 14:W:597:ARG:HH21    | 2.13                     | 0.53              |
| 14:W:649:LEU:HD23    | 15:J:575:ILE:CD1     | 1.96                     | 0.53              |
| 10:C:557:VAL:HG22    | 10:C:565:ARG:HE      | 1.73                     | 0.53              |
| 10:C:1076:TYR:O      | 10:C:1077:ALA:C      | 2.49                     | 0.53              |
| 10:C:1378:LYS:HA     | 10:C:1381:ALA:HB2    | 1.89                     | 0.53              |
| 11:A16:124:ASN:HB2   | 18:B:1523:ARG:NH1    | 2.22                     | 0.53              |
| 11:A16:322:ARG:HH11  | 11:A16:351:PHE:HZ    | 1.56                     | 0.53              |
| 11:A16:686:VAL:O     | 11:A16:686:VAL:HG12  | 2.08                     | 0.53              |
| 11:A32:524:GLU:OE2   | 11:A32:530:TYR:CD2   | 2.60                     | 0.53              |
| 18:B:1045:LYS:HZ3    | 18:B:1100:LEU:CD2    | 2.10                     | 0.53              |
| 18:B:1679:ARG:O      | 18:B:1681:GLN:N      | 2.41                     | 0.53              |
| 18:B8:1101:TYR:HD2   | 18:B8:1132:TRP:CZ3   | 2.26                     | 0.53              |
| 18:B8:1571:HIS:CD2   | 24:D32:1405:GLY:O    | 2.61                     | 0.53              |
| 19:4:185:GLY:C       | 19:4:187:SER:N       | 2.66                     | 0.53              |
| 20:E:429:PRO:CG      | 24:D:69:VAL:CA       | 2.79                     | 0.53              |
| 21:H:255:LEU:HD13    | 23:J32:655:GLU:OE2   | 2.01                     | 0.53              |
| 21:H16:312:GLN:NE2   | 21:H16:316:ILE:HD11  | 2.21                     | 0.53              |
| 23:J16:678:GLY:O     | 23:J16:680:LEU:N     | 2.40                     | 0.53              |
| 24:D:22:ARG:HH21     | 24:D:659:LEU:HD21    | 1.73                     | 0.53              |
| 24:D:1284:ILE:CD1    | 24:D:1329:VAL:HG21   | 2.38                     | 0.53              |
| 10:C32:1121:ILE:HG23 | 10:C32:1133:ILE:HD11 | 1.89                     | 0.53              |
| 12:A48:512:VAL:HG12  | 12:A48:512:VAL:O     | 2.08                     | 0.53              |
| 1:R:983:ARG:HD3      | 24:D:1364:PRO:CA     | 2.36                     | 0.53              |
| 2:M8:256:HIS:NE2     | 2:M8:273:VAL:HG22    | 2.23                     | 0.53              |
| 2:M8:344:GLN:O       | 2:M8:345:ASP:C       | 2.44                     | 0.53              |
| 2:M8:810:LEU:HD22    | 2:M8:819:GLN:CB      | 2.38                     | 0.53              |
| 5:P:12:GLU:HG3       | 5:P:78:GLY:H         | 1.74                     | 0.53              |
| 6:O:120:LYS:HG3      | 10:C:1163:LEU:HD11   | 1.90                     | 0.53              |
| 7:Q:147:GLU:OE1      | 7:Q:159:VAL:CG1      | 2.56                     | 0.53              |
| 5:P8:566:PHE:HZ      | 5:P8:597:GLY:O       | 1.91                     | 0.53              |
| 5:P8:614:VAL:CA      | 5:P8:629:ARG:CZ      | 2.84                     | 0.53              |
| 5:P8:624:HIS:CE1     | 5:P8:660:ARG:NH2     | 2.76                     | 0.53              |
| 6:O8:173:VAL:CG2     | 6:O8:189:LEU:HD13    | 2.27                     | 0.53              |
| 7:Q8:147:GLU:OE1     | 7:Q8:159:VAL:CG1     | 2.56                     | 0.53              |
| 5:P16:624:HIS:CE1    | 5:P16:660:ARG:NH2    | 2.76                     | 0.53              |
| 9:K8:879:CYS:HB2     | 9:K8:900:TYR:CE2     | 2.44                     | 0.53              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:879:LEU:HD21  | 10:C24:944:MET:HG3   | 1.90                     | 0.53              |
| 10:C24:1121:ILE:HG23 | 10:C24:1133:ILE:HD11 | 1.89                     | 0.53              |
| 11:A40:234:TYR:CZ    | 11:A40:249:MET:HB3   | 2.43                     | 0.53              |
| 11:A40:311:ASN:HB3   | 11:A40:357:TYR:CD2   | 2.44                     | 0.53              |
| 11:A40:322:ARG:HH11  | 11:A40:351:PHE:HZ    | 1.57                     | 0.53              |
| 12:A:643:SER:HB2     | 12:A:663:LEU:CD2     | 2.39                     | 0.53              |
| 12:A:686:VAL:HG12    | 12:A:686:VAL:O       | 2.08                     | 0.53              |
| 14:W:714:LEU:HB3     | 10:C8:1568:ARG:NH2   | 2.23                     | 0.53              |
| 10:C:513:LEU:HD12    | 10:C:546:LEU:HD23    | 1.90                     | 0.53              |
| 10:C:637:TYR:CZ      | 10:C:642:GLU:OE2     | 2.61                     | 0.53              |
| 10:C:768:ARG:HH22    | 10:C:775:LYS:HG2     | 1.68                     | 0.53              |
| 10:C:1724:VAL:HG22   | 10:C:1736:ILE:CD1    | 2.38                     | 0.53              |
| 10:C8:275:ALA:CB     | 10:C8:326:LEU:HD12   | 2.37                     | 0.53              |
| 10:C8:297:GLN:OE1    | 10:C8:320:TRP:NE1    | 2.37                     | 0.53              |
| 10:C8:637:TYR:CZ     | 10:C8:642:GLU:OE2    | 2.61                     | 0.53              |
| 10:C8:898:GLN:HG3    | 10:C8:1138:GLU:HG3   | 1.89                     | 0.53              |
| 10:C8:898:GLN:CG     | 10:C8:1138:GLU:HG3   | 2.38                     | 0.53              |
| 11:A16:234:TYR:CZ    | 11:A16:249:MET:HB3   | 2.43                     | 0.53              |
| 11:A16:573:TYR:HE1   | 11:A16:589:TYR:CZ    | 2.26                     | 0.53              |
| 11:A32:354:ARG:HD3   | 11:A32:452:TRP:CE3   | 2.44                     | 0.53              |
| 11:A32:573:TYR:HE1   | 11:A32:589:TYR:CZ    | 2.26                     | 0.53              |
| 18:B:243:GLY:HA3     | 18:B:249:TYR:CE2     | 2.44                     | 0.53              |
| 18:B:514:THR:HG23    | 18:B:549:TRP:HZ3     | 1.68                     | 0.53              |
| 18:B:1783:VAL:O      | 18:B:1784:GLY:C      | 2.48                     | 0.53              |
| 18:B8:359:VAL:HG21   | 18:B8:405:TYR:CZ     | 2.43                     | 0.53              |
| 18:B8:1541:LEU:HD23  | 18:B8:1580:SER:OG    | 2.08                     | 0.53              |
| 20:E8:25:PRO:HG3     | 20:E8:237:ILE:CD1    | 2.37                     | 0.53              |
| 23:J8:718:GLN:CG     | 23:J8:737:TRP:CZ3    | 2.91                     | 0.53              |
| 21:H24:255:LEU:HD13  | 23:J24:655:GLU:OE2   | 2.01                     | 0.53              |
| 22:I16:289:LEU:CD2   | 22:I16:296:ARG:HH12  | 2.17                     | 0.53              |
| 10:C32:513:LEU:HD12  | 10:C32:546:LEU:HD23  | 1.90                     | 0.53              |
| 10:C32:615:GLU:HA    | 10:C32:619:LEU:HD12  | 1.89                     | 0.53              |
| 10:C32:1058:GLU:O    | 10:C32:1059:ALA:C    | 2.46                     | 0.53              |
| 1:R:1191:LYS:HB2     | 24:D:1453:GLU:CD     | 2.32                     | 0.53              |
| 1:R:1204:ASN:C       | 1:R:1206:GLN:N       | 2.66                     | 0.53              |
| 1:R:1328:LYS:CA      | 10:C:1173:LEU:CD2    | 2.85                     | 0.53              |
| 1:R:1347:HIS:CE1     | 1:R:1349:ARG:HB2     | 2.43                     | 0.53              |
| 2:M:256:HIS:NE2      | 2:M:273:VAL:HG22     | 2.23                     | 0.53              |
| 2:M8:832:PRO:HB2     | 2:M8:834:ASP:OD1     | 2.08                     | 0.53              |
| 1:R16:1349:ARG:CG    | 1:R16:1390:GLU:HB3   | 2.38                     | 0.53              |
| 2:M16:319:LYS:O      | 2:M16:323:SER:OG     | 2.25                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:M16:673:ASN:CG    | 2:M16:681:ALA:HB2   | 2.33                     | 0.53              |
| 5:P:347:GLY:O       | 5:P:370:LEU:HD21    | 2.08                     | 0.53              |
| 5:P:566:PHE:HZ      | 5:P:597:GLY:O       | 1.91                     | 0.53              |
| 7:Q:236:HIS:CG      | 7:Q:237:PRO:HD2     | 2.43                     | 0.53              |
| 7:Q8:236:HIS:CG     | 7:Q8:237:PRO:HD2    | 2.43                     | 0.53              |
| 9:K:1176:ASP:OD1    | 9:K:1251:HIS:NE2    | 2.40                     | 0.53              |
| 10:C16:758:GLN:NE2  | 10:C16:819:GLN:CG   | 2.69                     | 0.53              |
| 11:A24:782:PRO:C    | 11:A24:783:PHE:CD2  | 2.86                     | 0.53              |
| 10:C24:390:HIS:CG   | 10:C24:449:GLU:OE2  | 2.60                     | 0.53              |
| 10:C24:1234:ASP:CG  | 10:C24:1302:LYS:HZ2 | 2.11                     | 0.53              |
| 11:A40:354:ARG:HD3  | 11:A40:452:TRP:CE3  | 2.44                     | 0.53              |
| 11:A40:782:PRO:C    | 11:A40:783:PHE:CD2  | 2.86                     | 0.53              |
| 12:A:518:ILE:HD11   | 12:A:541:LEU:HD12   | 1.90                     | 0.53              |
| 12:A:707:LEU:CD1    | 12:A:767:ARG:HH22   | 2.17                     | 0.53              |
| 14:W:631:TYR:CE1    | 15:J:554:LEU:HD11   | 2.43                     | 0.53              |
| 10:C:168:ARG:HH12   | 10:C:229:PRO:HA     | 1.70                     | 0.53              |
| 10:C:879:LEU:HD21   | 10:C:944:MET:CG     | 2.38                     | 0.53              |
| 10:C:925:GLU:OE1    | 10:C:973:LEU:HD23   | 2.08                     | 0.53              |
| 10:C:1009:GLN:C     | 10:C:1192:ARG:NH2   | 2.60                     | 0.53              |
| 10:C8:663:ILE:CG2   | 10:C8:667:ILE:HG23  | 2.38                     | 0.53              |
| 10:C8:1767:LEU:HD11 | 10:C8:1832:MET:CE   | 2.39                     | 0.53              |
| 11:A16:706:SER:HB2  | 24:D16:1398:ARG:NE  | 2.22                     | 0.53              |
| 11:A16:732:TYR:HE2  | 11:A16:738:VAL:HG11 | 1.74                     | 0.53              |
| 18:B:1507:ASN:OD1   | 18:B:1508:PRO:HD2   | 2.08                     | 0.53              |
| 18:B8:566:LYS:HE3   | 18:B8:574:GLU:CD    | 2.34                     | 0.53              |
| 18:B8:1058:ILE:CG2  | 18:B8:1154:ILE:HD11 | 2.39                     | 0.53              |
| 18:B8:1528:PRO:CA   | 18:B8:1531:TRP:NE1  | 2.64                     | 0.53              |
| 18:B8:1783:VAL:O    | 18:B8:1784:GLY:C    | 2.48                     | 0.53              |
| 19:4:126:ARG:NH1    | 19:4:134:LYS:O      | 2.36                     | 0.53              |
| 20:E:50:PHE:CZ      | 20:E:54:HIS:NE2     | 2.76                     | 0.53              |
| 19:48:185:GLY:C     | 19:48:187:SER:N     | 2.66                     | 0.53              |
| 20:E8:473:LEU:HD13  | 20:E8:514:PHE:HB3   | 1.89                     | 0.53              |
| 21:H8:312:GLN:HE22  | 22:I8:290:ASP:CG    | 2.17                     | 0.53              |
| 21:H24:179:GLU:O    | 21:H24:186:ARG:NH2  | 2.40                     | 0.53              |
| 22:I24:203:GLN:OE1  | 22:I24:209:TRP:CZ2  | 2.62                     | 0.53              |
| 23:J16:718:GLN:CG   | 23:J16:737:TRP:CZ3  | 2.91                     | 0.53              |
| 24:D:315:GLY:HA2    | 24:D16:839:GLU:OE2  | 2.07                     | 0.53              |
| 12:A48:322:ARG:HH11 | 12:A48:351:PHE:HZ   | 1.57                     | 0.53              |
| 1:R:1190:VAL:CG2    | 24:D:1457:SER:HA    | 2.36                     | 0.53              |
| 3:N:221:ASN:C       | 3:N:223:GLY:H       | 2.16                     | 0.53              |
| 1:R8:982:GLU:OE1    | 24:D40:1436:ARG:CD  | 2.56                     | 0.53              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:503:TYR:CE1     | 2:M8:507:LEU:HD11    | 2.43                     | 0.53              |
| 5:P:325:PHE:CE1      | 13:V:771:GLN:NE2     | 2.77                     | 0.53              |
| 7:Q:125:TYR:HD1      | 7:Q:167:GLY:HA2      | 1.72                     | 0.53              |
| 5:P8:165:PRO:O       | 5:P8:202:LEU:HD21    | 2.08                     | 0.53              |
| 5:P16:592:SER:C      | 5:P16:594:ILE:N      | 2.56                     | 0.53              |
| 9:K:1282:SER:C       | 9:K:1284:MET:N       | 2.64                     | 0.53              |
| 9:K8:1151:VAL:O      | 9:K8:1155:THR:HG23   | 2.08                     | 0.53              |
| 10:C16:1250:ALA:CB   | 10:C16:1309:ARG:HH12 | 2.15                     | 0.53              |
| 10:C16:1691:GLU:CD   | 23:J32:735:LYS:HA    | 2.33                     | 0.53              |
| 11:A24:322:ARG:HH11  | 11:A24:351:PHE:HZ    | 1.56                     | 0.53              |
| 11:A24:542:VAL:HG11  | 11:A24:596:THR:HG23  | 1.90                     | 0.53              |
| 10:C24:906:ARG:HB3   | 10:C24:907:PRO:HD2   | 1.89                     | 0.53              |
| 10:C24:1283:LEU:HD11 | 10:C24:1357:LEU:HD13 | 1.91                     | 0.53              |
| 10:C24:1642:TYR:CE1  | 10:C24:1646:LEU:HD11 | 2.43                     | 0.53              |
| 11:A40:696:ILE:HD11  | 11:A40:728:ILE:CD1   | 2.37                     | 0.53              |
| 12:A:234:TYR:CZ      | 12:A:249:MET:HB3     | 2.43                     | 0.53              |
| 14:W:631:TYR:CG      | 15:J:554:LEU:HD11    | 2.44                     | 0.53              |
| 10:C8:758:GLN:NE2    | 10:C8:819:GLN:CG     | 2.69                     | 0.53              |
| 10:C8:1541:PHE:CE1   | 10:C8:1649:LYS:CD    | 2.89                     | 0.53              |
| 11:A16:782:PRO:C     | 11:A16:783:PHE:CD2   | 2.86                     | 0.53              |
| 18:B:1175:ALA:HB2    | 18:B:1325:MET:HE2    | 1.90                     | 0.53              |
| 18:B:1637:VAL:HG21   | 24:D16:1405:GLY:H    | 1.73                     | 0.53              |
| 18:B8:1175:ALA:HB2   | 18:B8:1325:MET:HE2   | 1.90                     | 0.53              |
| 20:E:331:GLY:HA2     | 20:E:357:PHE:CZ      | 2.44                     | 0.53              |
| 19:48:209:CYS:SG     | 19:48:215:ILE:HD11   | 2.49                     | 0.53              |
| 21:H:240:ILE:CD1     | 22:I:174:GLN:OE1     | 2.57                     | 0.53              |
| 23:J16:734:PRO:O     | 23:J16:735:LYS:C     | 2.46                     | 0.53              |
| 10:C32:1285:VAL:HA   | 10:C32:1735:TYR:CE2  | 2.32                     | 0.53              |
| 2:M:191:TRP:CH2      | 2:M:222:ILE:HD11     | 2.43                     | 0.53              |
| 1:R16:1124:TRP:HZ2   | 4:T16:669:PRO:CG     | 2.13                     | 0.53              |
| 5:P:165:PRO:O        | 5:P:202:LEU:HD21     | 2.08                     | 0.53              |
| 7:Q:147:GLU:OE1      | 7:Q:159:VAL:HG11     | 2.07                     | 0.53              |
| 5:P8:16:PHE:CE1      | 6:O8:311:LEU:CG      | 2.91                     | 0.53              |
| 5:P16:486:CYS:HB2    | 5:P16:490:GLY:HA3    | 1.90                     | 0.53              |
| 9:K:923:ILE:HG21     | 9:K:929:ARG:HH21     | 1.71                     | 0.53              |
| 9:K:1245:GLU:HG3     | 9:K:1262:LEU:HD21    | 1.90                     | 0.53              |
| 9:K8:749:VAL:HG13    | 9:K8:752:MET:HE3     | 1.91                     | 0.53              |
| 9:K8:792:LEU:HD11    | 9:K8:849:LEU:HD22    | 1.91                     | 0.53              |
| 10:C16:325:MET:HE1   | 10:C16:352:LEU:HD21  | 1.90                     | 0.53              |
| 10:C16:1121:ILE:HG23 | 10:C16:1133:ILE:HD11 | 1.89                     | 0.53              |
| 10:C16:1333:HIS:CE1  | 10:C16:1337:LEU:HD23 | 2.38                     | 0.53              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A24:212:LYS:HE3   | 11:A24:585:MET:HE3  | 1.76                     | 0.53              |
| 11:A24:471:ASN:HD21  | 24:D16:1149:VAL:HB  | 1.72                     | 0.53              |
| 11:A24:518:ILE:HD11  | 11:A24:541:LEU:HD12 | 1.90                     | 0.53              |
| 11:A24:696:ILE:HD11  | 11:A24:728:ILE:CD1  | 2.37                     | 0.53              |
| 10:C24:182:ASP:CB    | 10:C24:183:PRO:CD   | 2.84                     | 0.53              |
| 11:A40:288:HIS:CB    | 11:A40:354:ARG:NH1  | 2.71                     | 0.53              |
| 11:A40:742:GLU:O     | 11:A40:746:VAL:HG23 | 2.09                     | 0.53              |
| 11:A16:86:LEU:HD23   | 22:I:301:LEU:HD23   | 1.90                     | 0.53              |
| 11:A32:20:LEU:HD11   | 21:H24:346:THR:HG23 | 1.91                     | 0.53              |
| 18:B8:86:LYS:CE      | 18:B8:123:LEU:CD1   | 2.86                     | 0.53              |
| 19:4:251:ARG:HH21    | 19:4:254:LEU:CD2    | 2.19                     | 0.53              |
| 21:H24:312:GLN:HE22  | 22:I24:290:ASP:CG   | 2.17                     | 0.53              |
| 22:I16:332:MET:SD    | 23:J16:732:MET:HE1  | 2.48                     | 0.53              |
| 24:D8:1170:VAL:HG22  | 24:D8:1232:VAL:CG2  | 2.38                     | 0.53              |
| 24:D24:22:ARG:HH21   | 24:D24:659:LEU:HD21 | 1.73                     | 0.53              |
| 24:D32:1170:VAL:HG22 | 24:D32:1232:VAL:CG2 | 2.38                     | 0.53              |
| 10:C32:453:LEU:HB3   | 10:C32:486:LEU:HD21 | 1.90                     | 0.53              |
| 12:A48:311:ASN:HB3   | 12:A48:357:TYR:CD2  | 2.44                     | 0.53              |
| 12:A48:518:ILE:HD11  | 12:A48:541:LEU:HD12 | 1.90                     | 0.53              |
| 1:R:1379:GLN:NE2     | 1:R:1416:TYR:CE1    | 2.75                     | 0.53              |
| 1:R:1428:VAL:CB      | 6:O:165:LYS:HZ2     | 2.22                     | 0.53              |
| 2:M:251:HIS:NE2      | 2:M:273:VAL:HG21    | 2.23                     | 0.53              |
| 2:M16:339:GLU:C      | 2:M16:341:ASP:H     | 2.16                     | 0.53              |
| 2:M16:544:LEU:HD11   | 2:M16:586:ALA:HB1   | 1.91                     | 0.53              |
| 5:P:43:TRP:HH2       | 5:P:76:LEU:CD1      | 2.21                     | 0.53              |
| 5:P:401:ARG:NH2      | 5:P:404:ILE:CB      | 2.72                     | 0.53              |
| 5:P:607:PHE:CE2      | 5:P:611:LEU:HD12    | 2.44                     | 0.53              |
| 5:P8:193:VAL:HG22    | 5:P8:364:VAL:HG13   | 1.89                     | 0.53              |
| 5:P8:607:PHE:CE2     | 5:P8:611:LEU:HD12   | 2.44                     | 0.53              |
| 5:P8:611:LEU:HA      | 5:P8:629:ARG:HE     | 1.70                     | 0.53              |
| 7:Q16:327:LEU:HD11   | 7:Q16:358:PHE:HE1   | 1.69                     | 0.53              |
| 8:L16:851:PRO:HG2    | 9:K16:1283:PRO:CA   | 2.25                     | 0.53              |
| 9:K:792:LEU:CD2      | 9:K:849:LEU:HD22    | 2.38                     | 0.53              |
| 9:K8:585:GLU:HA      | 9:K8:622:VAL:HG13   | 1.91                     | 0.53              |
| 9:K8:879:CYS:CB      | 9:K8:900:TYR:CE2    | 2.91                     | 0.53              |
| 10:C16:26:ARG:NH2    | 10:C16:151:LEU:HB2  | 2.24                     | 0.53              |
| 10:C16:453:LEU:HB3   | 10:C16:486:LEU:HD21 | 1.90                     | 0.53              |
| 10:C16:547:VAL:HG21  | 10:C16:587:TYR:HD2  | 1.73                     | 0.53              |
| 10:C16:1480:PHE:CD1  | 24:D8:1407:PHE:HD2  | 2.26                     | 0.53              |
| 10:C16:1767:LEU:HD11 | 10:C16:1832:MET:CE  | 2.39                     | 0.53              |
| 10:C24:453:LEU:HB3   | 10:C24:486:LEU:HD21 | 1.90                     | 0.53              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:557:VAL:HG22 | 10:C24:565:ARG:NE    | 2.24                     | 0.53              |
| 11:A40:86:LEU:HD23  | 22:I16:301:LEU:HD23  | 1.90                     | 0.53              |
| 11:A40:736:PRO:CB   | 24:D32:871:ARG:NH1   | 2.71                     | 0.53              |
| 12:A:742:GLU:O      | 12:A:746:VAL:HG23    | 2.09                     | 0.53              |
| 13:V:882:VAL:C      | 13:V:884:ASN:N       | 2.67                     | 0.53              |
| 13:V:910:GLU:N      | 14:W:787:MET:HE3     | 2.23                     | 0.53              |
| 14:W:220:TYR:CZ     | 14:W:242:THR:HG21    | 2.44                     | 0.53              |
| 10:C8:1094:LEU:HD21 | 10:C8:1203:MET:HB3   | 1.91                     | 0.53              |
| 11:A16:9:GLY:HA3    | 21:H:339:GLN:HE22    | 1.74                     | 0.53              |
| 11:A16:20:LEU:HD11  | 21:H:346:THR:HG23    | 1.91                     | 0.53              |
| 11:A16:90:PHE:HB3   | 18:B:1800:ARG:CZ     | 2.25                     | 0.53              |
| 18:B:152:HIS:CB     | 18:B:163:ILE:CD1     | 2.87                     | 0.53              |
| 18:B:195:MET:HE2    | 18:B:199:LEU:HD23    | 0.59                     | 0.53              |
| 18:B:1101:TYR:HD2   | 18:B:1132:TRP:CZ3    | 2.26                     | 0.53              |
| 18:B:1911:LEU:CB    | 18:B:1960:LEU:CD1    | 2.86                     | 0.53              |
| 18:B8:187:LEU:HD22  | 18:B8:251:PHE:HE2    | 1.71                     | 0.53              |
| 18:B8:856:LEU:CD2   | 18:B8:860:HIS:HB3    | 2.38                     | 0.53              |
| 18:B8:1507:ASN:OD1  | 18:B8:1508:PRO:HD2   | 2.08                     | 0.53              |
| 18:B8:1911:LEU:HB2  | 18:B8:1960:LEU:HD12  | 1.91                     | 0.53              |
| 19:48:117:ILE:CG1   | 19:48:150:LEU:HD23   | 2.39                     | 0.53              |
| 20:E8:345:LEU:CD2   | 24:D40:123:ALA:HB2   | 2.33                     | 0.53              |
| 21:H24:240:ILE:CD1  | 22:I24:174:GLN:OE1   | 2.57                     | 0.53              |
| 21:H24:322:LEU:HD22 | 22:I24:300:LEU:HG    | 1.89                     | 0.53              |
| 24:D:403:ARG:HD3    | 24:D16:744:LEU:O     | 2.08                     | 0.53              |
| 10:C32:1642:TYR:CE1 | 10:C32:1646:LEU:HD11 | 2.43                     | 0.53              |
| 12:A48:573:TYR:HE1  | 12:A48:589:TYR:CZ    | 2.26                     | 0.53              |
| 1:R:1349:ARG:CG     | 1:R:1390:GLU:HB3     | 2.38                     | 0.53              |
| 1:R:1449:TRP:HZ2    | 2:M:161:ASP:O        | 1.83                     | 0.53              |
| 2:M:247:PRO:HD3     | 2:M:290:ILE:HG21     | 1.89                     | 0.53              |
| 2:M:810:LEU:HD22    | 2:M:819:GLN:CB       | 2.38                     | 0.53              |
| 2:M8:254:LEU:O      | 2:M8:256:HIS:ND1     | 2.42                     | 0.53              |
| 1:R16:1225:PHE:CE1  | 1:R16:1247:PRO:HB3   | 2.40                     | 0.53              |
| 2:M16:503:TYR:CE1   | 2:M16:507:LEU:HD11   | 2.43                     | 0.53              |
| 2:M16:810:LEU:HD22  | 2:M16:819:GLN:CB     | 2.38                     | 0.53              |
| 7:Q:265:VAL:HG11    | 7:Q:271:ALA:CB       | 2.38                     | 0.53              |
| 5:P8:12:GLU:HG3     | 5:P8:78:GLY:H        | 1.73                     | 0.53              |
| 7:Q8:151:VAL:HG12   | 7:Q8:157:VAL:HG22    | 1.91                     | 0.53              |
| 5:P16:43:TRP:HH2    | 5:P16:76:LEU:CD1     | 2.21                     | 0.53              |
| 5:P16:624:HIS:HE1   | 5:P16:660:ARG:NH2    | 2.06                     | 0.53              |
| 9:K:950:LYS:HE3     | 9:K:977:GLU:CB       | 2.37                     | 0.53              |
| 9:K:1153:ALA:C      | 9:K:1220:ASN:ND2     | 2.63                     | 0.53              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:169:GLN:O     | 10:C16:173:THR:OG1  | 2.23                     | 0.53              |
| 10:C16:390:HIS:CE1   | 10:C16:449:GLU:CG   | 2.92                     | 0.53              |
| 11:A24:354:ARG:HD3   | 11:A24:452:TRP:CE3  | 2.44                     | 0.53              |
| 10:C24:275:ALA:CB    | 10:C24:326:LEU:HD12 | 2.37                     | 0.53              |
| 10:C24:325:MET:HE1   | 10:C24:352:LEU:HD21 | 1.90                     | 0.53              |
| 10:C24:390:HIS:CB    | 10:C24:452:LEU:HD23 | 2.36                     | 0.53              |
| 10:C24:399:HIS:ND1   | 10:C24:400:PRO:HD2  | 2.24                     | 0.53              |
| 10:C24:520:TYR:OH    | 10:C24:542:ASP:OD2  | 2.23                     | 0.53              |
| 10:C24:925:GLU:OE1   | 10:C24:973:LEU:HD23 | 2.08                     | 0.53              |
| 10:C24:1767:LEU:HD11 | 10:C24:1832:MET:CE  | 2.39                     | 0.53              |
| 11:A40:542:VAL:HG11  | 11:A40:596:THR:HG23 | 1.90                     | 0.53              |
| 13:V:814:MET:HE3     | 13:V:824:TRP:HZ2    | 1.72                     | 0.53              |
| 10:C:399:HIS:ND1     | 10:C:400:PRO:HD2    | 2.24                     | 0.53              |
| 10:C8:699:HIS:O      | 10:C8:703:SER:OG    | 2.24                     | 0.53              |
| 11:A16:311:ASN:HB3   | 11:A16:357:TYR:CD2  | 2.44                     | 0.53              |
| 11:A32:448:GLU:OE1   | 17:F24:61:THR:HB    | 2.08                     | 0.53              |
| 18:B:51:LEU:HD13     | 18:B:139:ARG:HH21   | 1.74                     | 0.53              |
| 18:B:359:VAL:HG21    | 18:B:405:TYR:CZ     | 2.43                     | 0.53              |
| 18:B:1058:ILE:CG2    | 18:B:1154:ILE:HD11  | 2.39                     | 0.53              |
| 18:B:1528:PRO:CA     | 18:B:1531:TRP:NE1   | 2.64                     | 0.53              |
| 18:B8:243:GLY:HA3    | 18:B8:249:TYR:CE2   | 2.44                     | 0.53              |
| 19:4:15:ILE:HD12     | 19:4:20:ILE:CD1     | 2.37                     | 0.53              |
| 19:4:31:GLN:OE1      | 19:4:41:VAL:CG2     | 2.57                     | 0.53              |
| 19:4:362:ALA:N       | 19:4:417:ASP:OD2    | 2.34                     | 0.53              |
| 20:E8:331:GLY:HA2    | 20:E8:357:PHE:CZ    | 2.44                     | 0.53              |
| 21:H:291:VAL:HG11    | 23:J32:657:GLU:HB3  | 1.91                     | 0.53              |
| 21:H24:291:VAL:HG11  | 23:J24:657:GLU:HB3  | 1.91                     | 0.53              |
| 23:J16:682:ALA:C     | 23:J16:684:ASP:H    | 2.15                     | 0.53              |
| 24:D8:1284:ILE:CD1   | 24:D8:1329:VAL:HG21 | 2.38                     | 0.53              |
| 24:D32:642:VAL:CG2   | 24:D40:631:ARG:NE   | 2.69                     | 0.53              |
| 10:C32:668:ALA:O     | 10:C32:704:MET:HE1  | 2.08                     | 0.53              |
| 1:R:1033:LYS:CE      | 24:D:1436:ARG:NE    | 2.71                     | 0.53              |
| 1:R:1379:GLN:HE22    | 1:R:1416:TYR:HE1    | 1.57                     | 0.53              |
| 3:N:218:TRP:CZ3      | 3:N:229:ILE:HD11    | 2.42                     | 0.53              |
| 1:R8:982:GLU:HG3     | 24:D40:1436:ARG:HE  | 1.73                     | 0.53              |
| 1:R8:1379:GLN:NE2    | 1:R8:1416:TYR:CE1   | 2.75                     | 0.53              |
| 2:M8:627:TYR:CD1     | 2:M8:627:TYR:C      | 2.84                     | 0.53              |
| 1:R16:1347:HIS:CE1   | 1:R16:1349:ARG:HB2  | 2.43                     | 0.53              |
| 2:M16:256:HIS:NE2    | 2:M16:273:VAL:HG22  | 2.23                     | 0.53              |
| 2:M16:416:VAL:CG1    | 8:L16:394:ALA:O     | 2.56                     | 0.53              |
| 6:O:125:VAL:HG23     | 6:O:175:TRP:CZ2     | 2.43                     | 0.53              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 7:Q:151:VAL:HG12     | 7:Q:157:VAL:HG22    | 1.91                     | 0.53              |
| 5:P8:101:LEU:CD2     | 5:P8:133:TYR:CZ     | 2.70                     | 0.53              |
| 6:O8:105:ASN:HD21    | 6:O8:134:ARG:HH22   | 1.57                     | 0.53              |
| 7:Q8:297:VAL:HG21    | 7:Q8:318:GLU:OE1    | 2.08                     | 0.53              |
| 5:P16:193:VAL:HG22   | 5:P16:364:VAL:HG13  | 1.89                     | 0.53              |
| 5:P16:310:ARG:NH1    | 5:P16:372:PRO:HG3   | 2.22                     | 0.53              |
| 7:Q16:297:VAL:HG21   | 7:Q16:318:GLU:OE1   | 2.08                     | 0.53              |
| 8:L8:1058:ILE:CG2    | 9:K8:1083:ILE:HD11  | 2.37                     | 0.53              |
| 8:L16:1041:SER:HB2   | 8:L16:1054:HIS:CE1  | 2.34                     | 0.53              |
| 9:K:923:ILE:HG22     | 9:K:929:ARG:NH2     | 2.24                     | 0.53              |
| 9:K:1151:VAL:O       | 9:K:1155:THR:HG23   | 2.08                     | 0.53              |
| 9:K8:1153:ALA:HA     | 9:K8:1220:ASN:ND2   | 2.24                     | 0.53              |
| 10:C16:11:VAL:HG13   | 10:C16:15:LEU:HD12  | 1.91                     | 0.53              |
| 10:C16:1548:ILE:HG12 | 24:D8:1407:PHE:CE2  | 2.21                     | 0.53              |
| 11:A24:736:PRO:HB2   | 24:D16:871:ARG:CZ   | 2.37                     | 0.53              |
| 10:C24:11:VAL:HG13   | 10:C24:15:LEU:HD12  | 1.91                     | 0.53              |
| 10:C24:26:ARG:NH2    | 10:C24:151:LEU:HB2  | 2.23                     | 0.53              |
| 11:A40:156:MET:CG    | 11:A40:555:HIS:NE2  | 2.38                     | 0.53              |
| 10:C:16:LEU:HD21     | 10:C:139:ARG:NH1    | 2.24                     | 0.53              |
| 10:C:547:VAL:HG21    | 10:C:587:TYR:HD2    | 1.73                     | 0.53              |
| 10:C8:11:VAL:HG13    | 10:C8:15:LEU:HD12   | 1.91                     | 0.53              |
| 10:C8:586:PRO:CD     | 10:C8:650:ARG:HH12  | 2.10                     | 0.53              |
| 10:C8:615:GLU:HA     | 10:C8:619:LEU:HD12  | 1.89                     | 0.53              |
| 10:C8:668:ALA:O      | 10:C8:704:MET:HE1   | 2.08                     | 0.53              |
| 10:C8:1255:GLN:OE1   | 16:A8:109:HIS:CE1   | 2.62                     | 0.53              |
| 10:C8:1553:VAL:HG23  | 10:C8:1592:VAL:HG12 | 1.91                     | 0.53              |
| 10:C8:1642:TYR:CE1   | 10:C8:1646:LEU:HD11 | 2.43                     | 0.53              |
| 10:C8:1767:LEU:HD12  | 10:C8:1832:MET:HE3  | 1.91                     | 0.53              |
| 10:C8:1812:GLU:HG3   | 10:C8:1819:LEU:HD12 | 1.91                     | 0.53              |
| 11:A16:153:ARG:NH1   | 18:B:1846:GLU:OE1   | 2.38                     | 0.53              |
| 11:A32:440:LEU:CG    | 11:A32:443:LEU:HD11 | 2.39                     | 0.53              |
| 18:B:497:PHE:CE1     | 18:B:512:VAL:HG11   | 2.44                     | 0.53              |
| 18:B:690:TRP:HH2     | 18:B:787:VAL:CG2    | 2.18                     | 0.53              |
| 18:B8:135:TYR:CZ     | 18:B8:139:ARG:HD2   | 2.43                     | 0.53              |
| 19:4:419:PHE:CE2     | 19:4:424:LEU:HD11   | 2.44                     | 0.53              |
| 23:J32:686:MET:HG2   | 23:J32:690:ASP:CB   | 2.39                     | 0.53              |
| 21:H8:253:ARG:NE     | 23:J8:621:GLU:OE2   | 2.38                     | 0.53              |
| 21:H8:338:MET:HE3    | 23:J8:692:VAL:CG2   | 2.38                     | 0.53              |
| 22:I8:300:LEU:HD11   | 23:J8:689:LEU:HD21  | 1.91                     | 0.53              |
| 21:H24:280:LEU:HD13  | 22:I24:263:LEU:HD23 | 1.90                     | 0.53              |
| 23:J24:686:MET:HG2   | 23:J24:690:ASP:CB   | 2.39                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 21:H16:291:VAL:HG11 | 23:J16:657:GLU:HB3  | 1.91                     | 0.53              |
| 24:D8:22:ARG:HH21   | 24:D8:659:LEU:HD21  | 1.73                     | 0.53              |
| 10:C32:452:LEU:H    | 10:C32:452:LEU:CD2  | 2.18                     | 0.53              |
| 10:C32:586:PRO:CD   | 10:C32:650:ARG:HH12 | 2.10                     | 0.53              |
| 1:R:1328:LYS:HE3    | 10:C:1177:ARG:CD    | 2.38                     | 0.53              |
| 2:M16:627:TYR:CE2   | 3:N16:166:ALA:N     | 2.77                     | 0.53              |
| 5:P:582:GLU:HG2     | 5:P:605:ARG:HG3     | 1.91                     | 0.53              |
| 6:O:5:MET:HE2       | 6:O:46:PHE:CE2      | 2.44                     | 0.53              |
| 6:O16:5:MET:HE2     | 6:O16:46:PHE:CE2    | 2.44                     | 0.53              |
| 9:K:1153:ALA:HA     | 9:K:1220:ASN:ND2    | 2.24                     | 0.53              |
| 9:K8:1180:TRP:CD1   | 9:K8:1261:MET:CE    | 2.80                     | 0.53              |
| 10:C16:1619:PRO:O   | 10:C16:1621:LYS:N   | 2.36                     | 0.53              |
| 11:A24:323:LEU:CD2  | 17:F:74:ILE:HD12    | 2.36                     | 0.53              |
| 10:C24:879:LEU:HD21 | 10:C24:944:MET:CG   | 2.38                     | 0.53              |
| 10:C24:1009:GLN:C   | 10:C24:1192:ARG:NH2 | 2.60                     | 0.53              |
| 10:C24:1255:GLN:OE1 | 11:A40:109:HIS:CE1  | 2.62                     | 0.53              |
| 11:A40:66:LEU:HB2   | 22:I16:323:GLU:OE2  | 2.09                     | 0.53              |
| 11:A40:448:GLU:OE1  | 17:F16:61:THR:HB    | 2.08                     | 0.53              |
| 11:A40:518:ILE:HD11 | 11:A40:541:LEU:HD12 | 1.90                     | 0.53              |
| 11:A40:573:TYR:HE1  | 11:A40:589:TYR:CZ   | 2.26                     | 0.53              |
| 10:C:37:PHE:HB3     | 10:C:38:PRO:HD3     | 1.91                     | 0.53              |
| 11:A32:9:GLY:HA3    | 21:H24:339:GLN:HE22 | 1.74                     | 0.53              |
| 11:A32:703:ALA:C    | 24:D32:1398:ARG:NH1 | 2.66                     | 0.53              |
| 18:B:1161:LEU:HD21  | 18:B:1403:ILE:CD1   | 2.37                     | 0.53              |
| 18:B:1541:LEU:HD23  | 18:B:1580:SER:OG    | 2.08                     | 0.53              |
| 18:B8:152:HIS:CB    | 18:B8:163:ILE:CD1   | 2.87                     | 0.53              |
| 19:4:117:ILE:CG1    | 19:4:150:LEU:HD23   | 2.39                     | 0.53              |
| 19:48:419:PHE:CE2   | 19:48:424:LEU:HD11  | 2.44                     | 0.53              |
| 21:H:322:LEU:HD22   | 22:I:300:LEU:HG     | 1.89                     | 0.53              |
| 22:I24:193:GLU:OE1  | 22:I24:197:ARG:NH2  | 2.42                     | 0.53              |
| 23:J24:718:GLN:CG   | 23:J24:737:TRP:CZ3  | 2.91                     | 0.53              |
| 22:I16:300:LEU:HD11 | 23:J16:689:LEU:HD21 | 1.91                     | 0.53              |
| 24:D8:816:VAL:O     | 24:D8:824:LYS:HE3   | 2.09                     | 0.53              |
| 10:C32:297:GLN:OE1  | 10:C32:320:TRP:NE1  | 2.37                     | 0.53              |
| 10:C32:619:LEU:CB   | 10:C32:620:PRO:HD2  | 2.23                     | 0.53              |
| 10:C32:1255:GLN:OE1 | 12:A48:109:HIS:CE1  | 2.62                     | 0.53              |
| 12:A48:440:LEU:HB2  | 12:A48:443:LEU:HD11 | 1.75                     | 0.53              |
| 2:M8:665:HIS:O      | 2:M8:684:GLN:NE2    | 2.41                     | 0.53              |
| 2:M16:254:LEU:O     | 2:M16:256:HIS:ND1   | 2.42                     | 0.53              |
| 2:M16:339:GLU:CD    | 4:T8:638:SER:O      | 2.51                     | 0.53              |
| 2:M16:340:GLU:HG2   | 4:T8:638:SER:OG     | 2.09                     | 0.53              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M16:417:ARG:HB2    | 8:L16:298:PHE:CE2    | 2.39                     | 0.53              |
| 2:M16:627:TYR:CD2    | 3:N16:166:ALA:O      | 2.61                     | 0.53              |
| 5:P:401:ARG:HH21     | 5:P:404:ILE:CB       | 2.22                     | 0.53              |
| 5:P:624:HIS:HE1      | 5:P:660:ARG:NH2      | 2.06                     | 0.53              |
| 7:Q:244:ILE:HG23     | 7:Q:289:TYR:CZ       | 2.44                     | 0.53              |
| 5:P8:206:SER:HG      | 5:P8:207:HIS:CE1     | 2.22                     | 0.53              |
| 5:P16:451:LYS:HD3    | 6:O16:312:ASN:O      | 2.08                     | 0.53              |
| 5:P16:566:PHE:HZ     | 5:P16:597:GLY:O      | 1.91                     | 0.53              |
| 9:K:730:SER:OG       | 9:K:735:ASP:OD1      | 2.17                     | 0.53              |
| 9:K:1048:GLN:HG3     | 9:K:1074:ARG:NH2     | 2.21                     | 0.53              |
| 9:K8:1245:GLU:HG3    | 9:K8:1262:LEU:HD21   | 1.90                     | 0.53              |
| 9:K16:912:TYR:HB2    | 9:K16:957:ILE:HD11   | 1.91                     | 0.53              |
| 10:C16:8:VAL:HG23    | 10:C16:133:THR:HG1   | 1.73                     | 0.53              |
| 10:C16:553:LEU:HD23  | 10:C16:595:THR:HG23  | 1.91                     | 0.53              |
| 10:C16:1767:LEU:HD12 | 10:C16:1832:MET:HE3  | 1.91                     | 0.53              |
| 11:A24:686:VAL:O     | 11:A24:686:VAL:HG12  | 2.08                     | 0.53              |
| 11:A24:732:TYR:HE2   | 11:A24:738:VAL:HG11  | 1.74                     | 0.53              |
| 11:A24:742:GLU:O     | 11:A24:746:VAL:HG23  | 2.09                     | 0.53              |
| 11:A40:732:TYR:HE2   | 11:A40:738:VAL:HG11  | 1.74                     | 0.53              |
| 13:V:818:THR:CG2     | 13:V:824:TRP:NE1     | 2.69                     | 0.53              |
| 13:V:881:GLY:O       | 13:V:883:PRO:HD3     | 2.09                     | 0.53              |
| 10:C:453:LEU:HB3     | 10:C:486:LEU:HD21    | 1.90                     | 0.53              |
| 10:C:966:CYS:SG      | 10:C:1021:TRP:CZ3    | 2.97                     | 0.53              |
| 10:C8:37:PHE:HB3     | 10:C8:38:PRO:HD3     | 1.91                     | 0.53              |
| 11:A32:323:LEU:CD2   | 17:F24:74:ILE:HD12   | 2.36                     | 0.53              |
| 11:A32:732:TYR:HE2   | 11:A32:738:VAL:HG11  | 1.74                     | 0.53              |
| 11:A32:798:PHE:HE2   | 11:A32:809:VAL:HG21  | 1.73                     | 0.53              |
| 18:B:86:LYS:CE       | 18:B:123:LEU:CD1     | 2.86                     | 0.53              |
| 18:B:1783:VAL:HG21   | 18:B:1810:VAL:HG11   | 1.90                     | 0.53              |
| 18:B8:51:LEU:HD13    | 18:B8:139:ARG:HH21   | 1.74                     | 0.53              |
| 18:B8:370:TYR:CE1    | 18:B8:374:ILE:HD11   | 2.43                     | 0.53              |
| 19:4:209:CYS:SG      | 19:4:215:ILE:HD11    | 2.49                     | 0.53              |
| 19:48:100:ILE:CG2    | 19:48:102:LEU:CG     | 2.74                     | 0.53              |
| 22:I:203:GLN:OE1     | 22:I:209:TRP:CZ2     | 2.63                     | 0.53              |
| 24:D16:1170:VAL:HG22 | 24:D16:1232:VAL:CG2  | 2.38                     | 0.53              |
| 10:C32:1812:GLU:HG3  | 10:C32:1819:LEU:HD12 | 1.91                     | 0.53              |
| 12:A48:686:VAL:HG12  | 12:A48:686:VAL:O     | 2.08                     | 0.53              |
| 12:A48:707:LEU:CD1   | 12:A48:767:ARG:HH22  | 2.17                     | 0.53              |
| 2:M:851:LEU:HD21     | 4:T:653:GLN:CG       | 2.22                     | 0.52              |
| 3:N:43:ASN:HD22      | 10:C:503:THR:CG2     | 2.12                     | 0.52              |
| 1:R8:526:ASN:CA      | 1:R8:529:HIS:HE1     | 2.21                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R8:1449:TRP:HZ2    | 2:M8:161:ASP:O       | 1.83                     | 0.52              |
| 2:M8:625:HIS:ND1     | 3:N8:165:GLY:HA2     | 2.24                     | 0.52              |
| 1:R16:1242:SER:HG    | 1:R16:1244:LEU:HD12  | 1.74                     | 0.52              |
| 2:M16:640:TYR:O      | 2:M16:644:TRP:CD1    | 2.62                     | 0.52              |
| 6:O:201:SER:OG       | 6:O:232:LEU:HD21     | 2.09                     | 0.52              |
| 7:Q:181:ALA:HB3      | 7:Q:198:TYR:CE2      | 2.44                     | 0.52              |
| 5:P8:241:LEU:O       | 5:P8:369:TYR:OH      | 2.18                     | 0.52              |
| 9:K:806:LEU:CD1      | 9:K:874:VAL:HG11     | 2.39                     | 0.52              |
| 10:C16:668:ALA:O     | 10:C16:704:MET:HE1   | 2.08                     | 0.52              |
| 10:C16:1094:LEU:HD21 | 10:C16:1203:MET:HB3  | 1.91                     | 0.52              |
| 10:C16:1812:GLU:HG3  | 10:C16:1819:LEU:HD12 | 1.91                     | 0.52              |
| 11:A24:512:VAL:O     | 11:A24:512:VAL:HG12  | 2.08                     | 0.52              |
| 11:A24:798:PHE:HE2   | 11:A24:809:VAL:HG21  | 1.73                     | 0.52              |
| 10:C24:1767:LEU:HD12 | 10:C24:1832:MET:HE3  | 1.91                     | 0.52              |
| 10:C24:1801:SER:HB3  | 10:C24:1802:PRO:HD3  | 1.90                     | 0.52              |
| 11:A40:440:LEU:CG    | 11:A40:443:LEU:HD11  | 2.39                     | 0.52              |
| 11:A40:512:VAL:HG12  | 11:A40:512:VAL:O     | 2.08                     | 0.52              |
| 10:C:11:VAL:HG13     | 10:C:15:LEU:HD12     | 1.91                     | 0.52              |
| 10:C:1094:LEU:HD21   | 10:C:1203:MET:HB3    | 1.91                     | 0.52              |
| 10:C:1285:VAL:HA     | 10:C:1735:TYR:CE2    | 2.32                     | 0.52              |
| 10:C8:960:PHE:CZ     | 10:C8:1138:GLU:OE2   | 2.56                     | 0.52              |
| 10:C8:1076:TYR:O     | 10:C8:1077:ALA:C     | 2.49                     | 0.52              |
| 11:A16:66:LEU:HB2    | 22:I:323:GLU:OE2     | 2.09                     | 0.52              |
| 11:A32:148:LEU:HD13  | 18:B8:1956:ILE:CD1   | 2.37                     | 0.52              |
| 11:A32:311:ASN:HB3   | 11:A32:357:TYR:CD2   | 2.44                     | 0.52              |
| 18:B8:1129:LYS:C     | 18:B8:1131:THR:H     | 2.17                     | 0.52              |
| 18:B8:1587:ARG:HG3   | 18:B8:1650:TYR:CZ    | 2.44                     | 0.52              |
| 20:E:407:LEU:HD11    | 20:E:462:THR:HG23    | 1.91                     | 0.52              |
| 20:E8:174:GLY:HA3    | 20:E8:236:HIS:CE1    | 2.45                     | 0.52              |
| 22:I:193:GLU:OE1     | 22:I:197:ARG:NH2     | 2.42                     | 0.52              |
| 22:I16:193:GLU:OE1   | 22:I16:197:ARG:NH2   | 2.42                     | 0.52              |
| 24:D24:816:VAL:O     | 24:D24:824:LYS:HE3   | 2.09                     | 0.52              |
| 24:D32:816:VAL:O     | 24:D32:824:LYS:HE3   | 2.09                     | 0.52              |
| 10:C32:1283:LEU:HD11 | 10:C32:1357:LEU:HD13 | 1.91                     | 0.52              |
| 12:A48:234:TYR:CZ    | 12:A48:249:MET:HB3   | 2.43                     | 0.52              |
| 12:A48:354:ARG:HD3   | 12:A48:452:TRP:CE3   | 2.44                     | 0.52              |
| 12:A48:794:THR:C     | 12:A48:796:ASP:H     | 2.17                     | 0.52              |
| 2:M16:625:HIS:ND1    | 3:N16:165:GLY:HA2    | 2.24                     | 0.52              |
| 2:M16:741:SER:OG     | 2:M16:775:ARG:NH1    | 2.41                     | 0.52              |
| 5:P:12:GLU:C         | 5:P:14:VAL:H         | 2.15                     | 0.52              |
| 5:P8:101:LEU:CD2     | 5:P8:133:TYR:CD1     | 2.92                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:879:CYS:HB2      | 9:K:900:TYR:CE2      | 2.43                     | 0.52              |
| 10:C16:557:VAL:HG22  | 10:C16:565:ARG:NE    | 2.24                     | 0.52              |
| 10:C16:1255:GLN:OE1  | 11:A24:109:HIS:CE1   | 2.62                     | 0.52              |
| 11:A24:157:LEU:HD22  | 11:A24:523:LYS:NZ    | 2.24                     | 0.52              |
| 11:A24:311:ASN:HB3   | 11:A24:357:TYR:CD2   | 2.44                     | 0.52              |
| 10:C24:16:LEU:HD21   | 10:C24:139:ARG:NH1   | 2.24                     | 0.52              |
| 10:C24:417:LEU:CB    | 10:C24:472:ASN:HD22  | 2.12                     | 0.52              |
| 10:C24:1094:LEU:HD21 | 10:C24:1203:MET:HB3  | 1.91                     | 0.52              |
| 10:C24:1812:GLU:HG3  | 10:C24:1819:LEU:HD12 | 1.91                     | 0.52              |
| 12:A:311:ASN:HB3     | 12:A:357:TYR:CD2     | 2.44                     | 0.52              |
| 14:W:715:ASP:N       | 10:C8:1568:ARG:NH1   | 2.57                     | 0.52              |
| 10:C:1271:PHE:HD1    | 10:C:1273:GLY:H      | 1.54                     | 0.52              |
| 10:C:1283:LEU:HD11   | 10:C:1357:LEU:HD13   | 1.91                     | 0.52              |
| 10:C:1619:PRO:O      | 10:C:1621:LYS:N      | 2.36                     | 0.52              |
| 11:A32:11:THR:CG2    | 22:I24:162:GLN:NE2   | 2.67                     | 0.52              |
| 18:B8:34:GLN:N       | 18:B8:35:PRO:CD      | 2.72                     | 0.52              |
| 18:B8:1185:LYS:HE3   | 18:B8:1314:SER:OG    | 2.09                     | 0.52              |
| 18:B8:1799:VAL:C     | 18:B8:1801:GLY:N     | 2.66                     | 0.52              |
| 19:4:251:ARG:NH2     | 19:4:254:LEU:HD23    | 2.21                     | 0.52              |
| 19:4:304:ILE:HD11    | 19:4:359:ALA:HA      | 1.91                     | 0.52              |
| 19:48:31:GLN:OE1     | 19:48:41:VAL:CG2     | 2.57                     | 0.52              |
| 20:E8:407:LEU:HD11   | 20:E8:462:THR:HG23   | 1.91                     | 0.52              |
| 21:H16:240:ILE:CD1   | 22:I16:174:GLN:OE1   | 2.57                     | 0.52              |
| 24:D:816:VAL:O       | 24:D:824:LYS:HE3     | 2.09                     | 0.52              |
| 10:C32:925:GLU:OE1   | 10:C32:973:LEU:HD23  | 2.08                     | 0.52              |
| 10:C32:1280:VAL:CG2  | 10:C32:1731:HIS:ND1  | 2.72                     | 0.52              |
| 1:R:526:ASN:CA       | 1:R:529:HIS:HE1      | 2.21                     | 0.52              |
| 1:R:1182:PRO:C       | 1:R:1184:GLU:N       | 2.68                     | 0.52              |
| 1:R:1360:GLN:O       | 10:C:608:ASP:CB      | 2.56                     | 0.52              |
| 2:M8:191:TRP:CH2     | 2:M8:222:ILE:HD11    | 2.43                     | 0.52              |
| 1:R16:1175:TYR:CA    | 1:R16:1177:TRP:CZ3   | 2.79                     | 0.52              |
| 5:P:175:MET:CE       | 5:P:436:ALA:HB1      | 2.23                     | 0.52              |
| 6:O:105:ASN:HD21     | 6:O:134:ARG:HH22     | 1.57                     | 0.52              |
| 6:O8:5:MET:HE2       | 6:O8:46:PHE:CE2      | 2.44                     | 0.52              |
| 7:Q8:244:ILE:HG23    | 7:Q8:289:TYR:CZ      | 2.44                     | 0.52              |
| 7:Q16:151:VAL:HG12   | 7:Q16:157:VAL:HG22   | 1.91                     | 0.52              |
| 7:Q16:181:ALA:HB3    | 7:Q16:198:TYR:CE2    | 2.45                     | 0.52              |
| 8:L16:856:LEU:CD2    | 9:K16:1281:SER:CB    | 2.74                     | 0.52              |
| 8:L16:1062:ALA:HB2   | 9:K16:1083:ILE:CG1   | 2.39                     | 0.52              |
| 9:K:919:MET:SD       | 9:K:938:PHE:HD2      | 2.31                     | 0.52              |
| 9:K:923:ILE:CG2      | 9:K:929:ARG:NH2      | 2.72                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:1133:ILE:CG2     | 9:K:1166:LEU:HD23    | 2.39                     | 0.52              |
| 10:C16:390:HIS:CB    | 10:C16:452:LEU:CB    | 2.86                     | 0.52              |
| 10:C16:452:LEU:H     | 10:C16:452:LEU:CD2   | 2.18                     | 0.52              |
| 11:A24:440:LEU:CG    | 11:A24:443:LEU:HD11  | 2.39                     | 0.52              |
| 11:A40:464:GLY:C     | 11:A40:466:SER:H     | 2.18                     | 0.52              |
| 12:A:354:ARG:HD3     | 12:A:452:TRP:CE3     | 2.44                     | 0.52              |
| 12:A:573:TYR:HE1     | 12:A:589:TYR:CZ      | 2.26                     | 0.52              |
| 14:W:518:GLU:H       | 14:W:605:ASN:ND2     | 2.04                     | 0.52              |
| 10:C:1642:TYR:CE1    | 10:C:1646:LEU:HD11   | 2.43                     | 0.52              |
| 10:C:1767:LEU:HD12   | 10:C:1832:MET:HE3    | 1.91                     | 0.52              |
| 10:C8:26:ARG:NH2     | 10:C8:151:LEU:HB2    | 2.24                     | 0.52              |
| 10:C8:513:LEU:HD12   | 10:C8:546:LEU:HD23   | 1.90                     | 0.52              |
| 11:A16:273:ARG:NE    | 11:A16:479:LEU:HD23  | 2.19                     | 0.52              |
| 11:A32:66:LEU:HB2    | 22:I24:323:GLU:OE2   | 2.09                     | 0.52              |
| 11:A32:86:LEU:HD23   | 22:I24:301:LEU:HD23  | 1.90                     | 0.52              |
| 11:A32:90:PHE:CD2    | 18:B8:1788:ILE:CG1   | 2.93                     | 0.52              |
| 18:B:689:SER:C       | 18:B:691:SER:H       | 2.16                     | 0.52              |
| 18:B:1587:ARG:HG3    | 18:B:1650:TYR:CZ     | 2.44                     | 0.52              |
| 18:B8:817:CYS:CB     | 18:B8:885:ARG:HH12   | 2.08                     | 0.52              |
| 18:B8:846:SER:CB     | 18:B8:899:LYS:HZ3    | 2.07                     | 0.52              |
| 18:B8:1783:VAL:HG21  | 18:B8:1810:VAL:HG11  | 1.90                     | 0.52              |
| 21:H:228:LEU:HD11    | 23:J32:593:VAL:CG2   | 2.34                     | 0.52              |
| 21:H:269:PHE:CE1     | 22:I:205:ARG:CZ      | 2.90                     | 0.52              |
| 21:H:338:MET:HE3     | 23:J32:692:VAL:CG2   | 2.38                     | 0.52              |
| 23:J32:686:MET:HG2   | 23:J32:690:ASP:HB2   | 1.91                     | 0.52              |
| 23:J32:718:GLN:CG    | 23:J32:737:TRP:CZ3   | 2.91                     | 0.52              |
| 21:H8:269:PHE:CE1    | 22:I8:205:ARG:CZ     | 2.90                     | 0.52              |
| 23:J8:678:GLY:O      | 23:J8:680:LEU:N      | 2.40                     | 0.52              |
| 23:J24:686:MET:HG2   | 23:J24:690:ASP:HB2   | 1.91                     | 0.52              |
| 24:D:1:MET:SD        | 24:D:882:GLU:OE2     | 2.67                     | 0.52              |
| 10:C32:11:VAL:HG13   | 10:C32:15:LEU:HD12   | 1.91                     | 0.52              |
| 10:C32:168:ARG:HH12  | 10:C32:229:PRO:HA    | 1.70                     | 0.52              |
| 10:C32:553:LEU:HD23  | 10:C32:595:THR:HG23  | 1.91                     | 0.52              |
| 10:C32:1553:VAL:HG23 | 10:C32:1592:VAL:HG12 | 1.91                     | 0.52              |
| 12:A48:742:GLU:O     | 12:A48:746:VAL:HG23  | 2.09                     | 0.52              |
| 1:R:1424:LYS:HB3     | 6:O:107:SER:HB2      | 1.89                     | 0.52              |
| 3:N16:200:MET:HE3    | 3:N16:203:PHE:HD2    | 1.74                     | 0.52              |
| 5:P:16:PHE:CE1       | 6:O:311:LEU:HD21     | 2.45                     | 0.52              |
| 7:Q:114:ASP:O        | 7:Q:119:ALA:HA       | 2.10                     | 0.52              |
| 5:P8:643:PHE:C       | 5:P8:646:PRO:HD2     | 2.34                     | 0.52              |
| 6:O8:54:VAL:HG13     | 6:O8:85:TRP:CE2      | 2.45                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:16:PHE:CE1     | 6:O16:311:LEU:HD21   | 2.45                     | 0.52              |
| 8:L8:608:PHE:CD2     | 8:L8:635:MET:CG      | 2.92                     | 0.52              |
| 8:L8:1074:ARG:HD3    | 9:K8:1089:LYS:CD     | 2.39                     | 0.52              |
| 9:K:707:GLN:OE1      | 9:K:761:TYR:OH       | 2.22                     | 0.52              |
| 9:K16:975:MET:CG     | 9:K16:985:PHE:CE1    | 2.92                     | 0.52              |
| 10:C16:182:ASP:CB    | 10:C16:183:PRO:CD    | 2.84                     | 0.52              |
| 10:C16:1682:VAL:HG22 | 10:C16:1758:LEU:HD23 | 1.89                     | 0.52              |
| 11:A24:66:LEU:HB2    | 22:I8:323:GLU:OE2    | 2.09                     | 0.52              |
| 11:A24:448:GLU:OE1   | 17:F:61:THR:HB       | 2.09                     | 0.52              |
| 11:A24:794:THR:C     | 11:A24:796:ASP:H     | 2.17                     | 0.52              |
| 10:C24:1271:PHE:CD1  | 10:C24:1731:HIS:NE2  | 2.75                     | 0.52              |
| 11:A40:798:PHE:HE2   | 11:A40:809:VAL:HG21  | 1.73                     | 0.52              |
| 14:W:586:ILE:HG13    | 15:J:572:ASP:CB      | 2.39                     | 0.52              |
| 14:W:598:ILE:CG2     | 14:W:626:LEU:CD2     | 2.78                     | 0.52              |
| 10:C:653:TYR:CE1     | 10:C:679:ARG:HD2     | 2.44                     | 0.52              |
| 11:A16:464:GLY:C     | 11:A16:466:SER:H     | 2.18                     | 0.52              |
| 11:A16:703:ALA:C     | 24:D16:1398:ARG:NH1  | 2.67                     | 0.52              |
| 11:A32:464:GLY:C     | 11:A32:466:SER:H     | 2.18                     | 0.52              |
| 18:B:566:LYS:HE3     | 18:B:574:GLU:CD      | 2.33                     | 0.52              |
| 18:B8:112:GLU:CD     | 18:B8:130:MET:CE     | 2.83                     | 0.52              |
| 18:B8:277:GLU:OE2    | 18:B8:393:VAL:HG22   | 2.09                     | 0.52              |
| 18:B8:326:PRO:HB3    | 18:B8:371:PHE:CZ     | 2.45                     | 0.52              |
| 18:B8:1674:ASP:C     | 18:B8:1676:VAL:N     | 2.67                     | 0.52              |
| 20:E8:353:ILE:CD1    | 20:E8:413:PHE:HD2    | 1.61                     | 0.52              |
| 21:H:312:GLN:HE22    | 22:I:290:ASP:CG      | 2.17                     | 0.52              |
| 21:H:366:MET:HE3     | 22:I:332:MET:CE      | 2.32                     | 0.52              |
| 23:J32:686:MET:CE    | 23:J32:694:ARG:HH21  | 2.10                     | 0.52              |
| 21:H8:284:LEU:HD21   | 23:J8:650:GLN:HB3    | 1.92                     | 0.52              |
| 22:I8:131:ARG:CG     | 23:J8:557:ARG:HH22   | 2.11                     | 0.52              |
| 24:D40:22:ARG:HH21   | 24:D40:659:LEU:HD21  | 1.73                     | 0.52              |
| 24:D40:1101:HIS:C    | 24:D40:1134:GLN:OE1  | 2.52                     | 0.52              |
| 10:C32:653:TYR:CE1   | 10:C32:679:ARG:HD2   | 2.44                     | 0.52              |
| 12:A48:464:GLY:C     | 12:A48:466:SER:H     | 2.18                     | 0.52              |
| 1:R:1324:ASP:CG      | 10:C:1180:ILE:HB     | 2.33                     | 0.52              |
| 1:R:1326:GLY:C       | 10:C:1154:TRP:HE1    | 2.15                     | 0.52              |
| 1:R:1361:ALA:C       | 10:C:608:ASP:OD2     | 2.53                     | 0.52              |
| 3:N:97:HIS:HD2       | 3:N:99:PHE:CE1       | 2.28                     | 0.52              |
| 3:N:200:MET:HE3      | 3:N:203:PHE:HD2      | 1.74                     | 0.52              |
| 1:R16:1101:ARG:HH11  | 1:R16:1188:TYR:HE2   | 1.48                     | 0.52              |
| 2:M16:166:THR:H      | 2:M16:169:THR:HG1    | 1.50                     | 0.52              |
| 2:M16:627:TYR:CA     | 3:N16:167:LEU:HD12   | 2.39                     | 0.52              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 6:O8:119:ARG:NH2     | 6:O8:182:GLU:CA     | 2.57                     | 0.52              |
| 7:Q8:221:TRP:CD1     | 7:Q8:221:TRP:N      | 2.78                     | 0.52              |
| 5:P16:12:GLU:HG3     | 5:P16:78:GLY:H      | 1.74                     | 0.52              |
| 6:O16:201:SER:OG     | 6:O16:232:LEU:HD21  | 2.09                     | 0.52              |
| 10:C16:16:LEU:HD21   | 10:C16:139:ARG:NH1  | 2.24                     | 0.52              |
| 10:C16:286:ILE:HG21  | 10:C16:292:PHE:CE1  | 2.45                     | 0.52              |
| 11:A24:464:GLY:C     | 11:A24:466:SER:H    | 2.18                     | 0.52              |
| 11:A24:798:PHE:HZ    | 11:A24:847:ARG:NH1  | 2.01                     | 0.52              |
| 11:A40:489:PHE:CZ    | 17:F16:56:PRO:HA    | 2.45                     | 0.52              |
| 11:A40:686:VAL:O     | 11:A40:686:VAL:HG12 | 2.08                     | 0.52              |
| 12:A:464:GLY:C       | 12:A:466:SER:H      | 2.18                     | 0.52              |
| 10:C:1251:PHE:HZ     | 10:C:1319:ARG:HH12  | 1.39                     | 0.52              |
| 10:C8:643:LEU:HB3    | 10:C8:679:ARG:HH12  | 1.73                     | 0.52              |
| 10:C8:643:LEU:HG     | 10:C8:656:THR:OG1   | 2.09                     | 0.52              |
| 10:C8:879:LEU:HD21   | 10:C8:944:MET:HG3   | 1.90                     | 0.52              |
| 11:A16:354:ARG:HD3   | 11:A16:452:TRP:CE3  | 2.44                     | 0.52              |
| 11:A16:518:ILE:HD11  | 11:A16:541:LEU:HD12 | 1.91                     | 0.52              |
| 11:A32:257:GLN:CD    | 11:A32:263:ASP:OD1  | 2.51                     | 0.52              |
| 11:A32:518:ILE:HD11  | 11:A32:541:LEU:HD12 | 1.91                     | 0.52              |
| 11:A32:676:TYR:HE2   | 24:D32:1395:SER:C   | 2.15                     | 0.52              |
| 11:A32:711:ARG:HD3   | 24:D32:1398:ARG:HG3 | 1.89                     | 0.52              |
| 11:A32:794:THR:C     | 11:A32:796:ASP:H    | 2.18                     | 0.52              |
| 18:B:326:PRO:HB3     | 18:B:371:PHE:CZ     | 2.45                     | 0.52              |
| 18:B:1185:LYS:HE3    | 18:B:1314:SER:OG    | 2.09                     | 0.52              |
| 18:B8:846:SER:HG     | 18:B8:899:LYS:NZ    | 1.93                     | 0.52              |
| 18:B8:1161:LEU:CG    | 18:B8:1403:ILE:HD13 | 2.40                     | 0.52              |
| 18:B8:1438:LEU:HD13  | 18:B8:1462:LEU:CD1  | 2.40                     | 0.52              |
| 19:48:304:ILE:HD11   | 19:48:359:ALA:HA    | 1.91                     | 0.52              |
| 22:I8:199:PHE:CG     | 23:J8:620:MET:CG    | 2.93                     | 0.52              |
| 23:J16:686:MET:HG2   | 23:J16:690:ASP:CB   | 2.39                     | 0.52              |
| 24:D32:22:ARG:HH21   | 24:D32:659:LEU:HD21 | 1.73                     | 0.52              |
| 10:C32:664:ASN:HA    | 10:C32:667:ILE:HG12 | 1.91                     | 0.52              |
| 10:C32:879:LEU:HD21  | 10:C32:944:MET:CG   | 2.38                     | 0.52              |
| 10:C32:1297:HIS:NE2  | 10:C32:1372:ALA:CB  | 2.73                     | 0.52              |
| 10:C32:1624:LEU:HD23 | 10:C32:1628:SER:CB  | 2.37                     | 0.52              |
| 10:C32:1767:LEU:HD11 | 10:C32:1832:MET:CE  | 2.39                     | 0.52              |
| 2:M:627:TYR:HB3      | 3:N:167:LEU:CG      | 2.40                     | 0.52              |
| 2:M8:278:VAL:HG13    | 2:M8:326:GLN:HG3    | 1.91                     | 0.52              |
| 2:M8:625:HIS:HE2     | 3:N8:225:PRO:CB     | 2.23                     | 0.52              |
| 1:R16:1449:TRP:CZ3   | 2:M16:160:LEU:HD11  | 2.37                     | 0.52              |
| 2:M16:816:ARG:NH2    | 2:M16:849:LEU:HB3   | 2.25                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 4:T16:671:ILE:CD1    | 5:P16:698:GLY:CA     | 2.86                     | 0.52              |
| 5:P8:16:PHE:CE1      | 6:O8:311:LEU:HD21    | 2.45                     | 0.52              |
| 5:P8:214:LEU:HD21    | 5:P8:236:VAL:CG1     | 2.39                     | 0.52              |
| 6:O8:119:ARG:CG      | 6:O8:181:GLU:O       | 2.58                     | 0.52              |
| 5:P16:582:GLU:HG2    | 5:P16:605:ARG:HG3    | 1.91                     | 0.52              |
| 6:O16:119:ARG:CG     | 6:O16:181:GLU:O      | 2.58                     | 0.52              |
| 8:L:1096:GLU:OE1     | 9:K:996:MET:C        | 2.47                     | 0.52              |
| 9:K8:923:ILE:HG22    | 9:K8:929:ARG:NH2     | 2.24                     | 0.52              |
| 9:K8:955:TYR:CE2     | 9:K8:984:GLY:C       | 2.87                     | 0.52              |
| 10:C16:417:LEU:CB    | 10:C16:472:ASN:HD22  | 2.12                     | 0.52              |
| 10:C16:520:TYR:OH    | 10:C16:542:ASP:OD2   | 2.23                     | 0.52              |
| 10:C16:1271:PHE:CD1  | 10:C16:1731:HIS:NE2  | 2.75                     | 0.52              |
| 10:C16:1280:VAL:CG2  | 10:C16:1731:HIS:ND1  | 2.72                     | 0.52              |
| 10:C16:1283:LEU:HD11 | 10:C16:1357:LEU:HD13 | 1.91                     | 0.52              |
| 10:C16:1553:VAL:HG23 | 10:C16:1592:VAL:HG12 | 1.91                     | 0.52              |
| 10:C24:553:LEU:HD23  | 10:C24:595:THR:HG23  | 1.91                     | 0.52              |
| 11:A40:794:THR:C     | 11:A40:796:ASP:H     | 2.18                     | 0.52              |
| 12:A:212:LYS:HE3     | 12:A:585:MET:HE3     | 1.76                     | 0.52              |
| 12:A:785:HIS:CB      | 12:A:793:ALA:HB2     | 2.39                     | 0.52              |
| 14:W:806:GLU:OE2     | 15:J:716:ARG:NH2     | 2.38                     | 0.52              |
| 10:C:22:THR:HB       | 10:C:23:PRO:HD2      | 1.92                     | 0.52              |
| 10:C:1283:LEU:HD23   | 10:C:1287:MET:HE2    | 1.91                     | 0.52              |
| 10:C:1283:LEU:CD1    | 10:C:1357:LEU:CD1    | 2.88                     | 0.52              |
| 10:C:1767:LEU:HD11   | 10:C:1832:MET:CE     | 2.39                     | 0.52              |
| 10:C8:894:VAL:HG13   | 10:C8:960:PHE:HE2    | 1.72                     | 0.52              |
| 11:A16:742:GLU:O     | 11:A16:746:VAL:HG23  | 2.09                     | 0.52              |
| 11:A16:794:THR:C     | 11:A16:796:ASP:H     | 2.17                     | 0.52              |
| 18:B:1112:LYS:HZ1    | 21:H:327:SER:C       | 2.14                     | 0.52              |
| 18:B:1161:LEU:CG     | 18:B:1403:ILE:HD13   | 2.40                     | 0.52              |
| 18:B:1438:LEU:HD13   | 18:B:1462:LEU:CD1    | 2.40                     | 0.52              |
| 18:B8:187:LEU:CD2    | 18:B8:251:PHE:CE2    | 2.93                     | 0.52              |
| 19:4:185:GLY:O       | 19:4:187:SER:N       | 2.42                     | 0.52              |
| 20:E:32:PHE:O        | 20:E:36:PHE:HD2      | 1.93                     | 0.52              |
| 20:E:332:LEU:O       | 20:E:336:PHE:CD2     | 2.63                     | 0.52              |
| 19:48:252:ARG:HG2    | 19:48:281:TRP:HH2    | 1.67                     | 0.52              |
| 21:H:280:LEU:HD13    | 22:I:263:LEU:HD23    | 1.90                     | 0.52              |
| 21:H8:240:ILE:CD1    | 22:I8:174:GLN:OE1    | 2.57                     | 0.52              |
| 21:H8:280:LEU:HD13   | 22:I8:263:LEU:HD23   | 1.90                     | 0.52              |
| 21:H16:280:LEU:HD13  | 22:I16:263:LEU:HD23  | 1.90                     | 0.52              |
| 21:H16:312:GLN:HE22  | 22:I16:290:ASP:CG    | 2.17                     | 0.52              |
| 24:D:403:ARG:NH2     | 24:D:409:LEU:CD1     | 2.70                     | 0.52              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 24:D40:853:MET:CB    | 24:D40:925:ASP:OD2  | 2.57                     | 0.52              |
| 10:C32:452:LEU:HD23  | 10:C32:452:LEU:N    | 2.20                     | 0.52              |
| 10:C32:1767:LEU:HD12 | 10:C32:1832:MET:HE3 | 1.91                     | 0.52              |
| 2:M:254:LEU:O        | 2:M:256:HIS:ND1     | 2.42                     | 0.52              |
| 2:M:818:THR:O        | 2:M:821:THR:OG1     | 2.27                     | 0.52              |
| 2:M8:166:THR:C       | 2:M8:168:LEU:N      | 2.67                     | 0.52              |
| 1:R16:1379:GLN:HE22  | 1:R16:1416:TYR:HE1  | 1.57                     | 0.52              |
| 2:M16:627:TYR:HB3    | 3:N16:167:LEU:CG    | 2.39                     | 0.52              |
| 5:P:643:PHE:C        | 5:P:646:PRO:HD2     | 2.35                     | 0.52              |
| 7:Q8:295:SER:HB2     | 7:Q8:297:VAL:CG2    | 2.39                     | 0.52              |
| 7:Q16:219:GLY:C      | 7:Q16:221:TRP:CD1   | 2.88                     | 0.52              |
| 7:Q16:244:ILE:HG23   | 7:Q16:289:TYR:CZ    | 2.44                     | 0.52              |
| 9:K:916:LYS:HG3      | 9:K:919:MET:HE1     | 1.87                     | 0.52              |
| 9:K16:1232:LEU:HD22  | 9:K16:1265:ILE:CG2  | 2.40                     | 0.52              |
| 10:C16:399:HIS:ND1   | 10:C16:400:PRO:HD2  | 2.24                     | 0.52              |
| 10:C16:1286:MET:HE3  | 10:C16:1344:VAL:CG1 | 2.37                     | 0.52              |
| 10:C16:1724:VAL:HG22 | 10:C16:1736:ILE:CD1 | 2.38                     | 0.52              |
| 12:A:732:TYR:HE2     | 12:A:738:VAL:HG11   | 1.74                     | 0.52              |
| 10:C:26:ARG:NH2      | 10:C:151:LEU:HB2    | 2.24                     | 0.52              |
| 10:C:792:PHE:HD1     | 10:C:850:ARG:CZ     | 2.23                     | 0.52              |
| 10:C:1812:GLU:HG3    | 10:C:1819:LEU:HD12  | 1.91                     | 0.52              |
| 10:C8:1553:VAL:HG23  | 10:C8:1592:VAL:CG1  | 2.40                     | 0.52              |
| 11:A16:676:TYR:HE2   | 24:D16:1395:SER:C   | 2.17                     | 0.52              |
| 11:A32:742:GLU:O     | 11:A32:746:VAL:HG23 | 2.09                     | 0.52              |
| 18:B:112:GLU:CD      | 18:B:130:MET:CE     | 2.83                     | 0.52              |
| 18:B:187:LEU:CD2     | 18:B:251:PHE:CE2    | 2.93                     | 0.52              |
| 18:B:749:HIS:HA      | 18:B:752:TRP:CE2    | 2.45                     | 0.52              |
| 18:B:1911:LEU:HA     | 18:B:1960:LEU:CD1   | 2.40                     | 0.52              |
| 18:B8:749:HIS:HA     | 18:B8:752:TRP:CE2   | 2.45                     | 0.52              |
| 18:B8:1129:LYS:C     | 18:B8:1131:THR:N    | 2.68                     | 0.52              |
| 18:B8:1441:LEU:HA    | 18:B8:1444:LEU:HD12 | 1.92                     | 0.52              |
| 18:B8:1528:PRO:HA    | 18:B8:1531:TRP:CD1  | 2.42                     | 0.52              |
| 23:J8:686:MET:HG2    | 23:J8:690:ASP:HB2   | 1.91                     | 0.52              |
| 21:H16:258:MET:HG2   | 22:I16:261:PHE:CD1  | 2.45                     | 0.52              |
| 21:H16:284:LEU:HD21  | 23:J16:650:GLN:HB3  | 1.92                     | 0.52              |
| 1:R8:1112:LYS:HD3    | 5:P8:712:PHE:CZ     | 2.43                     | 0.52              |
| 6:O:43:SER:HA        | 7:Q:45:ASP:OD2      | 2.10                     | 0.52              |
| 6:O8:160:LEU:HG      | 6:O8:160:LEU:O      | 2.08                     | 0.52              |
| 6:O16:43:SER:HA      | 7:Q16:45:ASP:OD2    | 2.10                     | 0.52              |
| 6:O16:119:ARG:CZ     | 6:O16:182:GLU:HA    | 2.38                     | 0.52              |
| 8:L8:598:LEU:HD21    | 8:L8:627:ARG:NH1    | 2.24                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:806:LEU:CD1      | 9:K:874:VAL:HG12     | 2.37                     | 0.52              |
| 10:C16:557:VAL:CG2   | 10:C16:565:ARG:NH2   | 2.45                     | 0.52              |
| 10:C16:586:PRO:CD    | 10:C16:650:ARG:HH12  | 2.10                     | 0.52              |
| 10:C16:1297:HIS:NE2  | 10:C16:1372:ALA:CB   | 2.73                     | 0.52              |
| 10:C16:1547:LYS:HE2  | 24:D8:1405:GLY:CA    | 2.39                     | 0.52              |
| 11:A24:10:TRP:CH2    | 21:H8:338:MET:HE3    | 2.45                     | 0.52              |
| 11:A24:288:HIS:CE1   | 11:A24:292:ILE:HD11  | 2.45                     | 0.52              |
| 11:A24:573:TYR:HE1   | 11:A24:589:TYR:CZ    | 2.26                     | 0.52              |
| 11:A24:743:ARG:NH2   | 24:D16:699:HIS:CD2   | 2.75                     | 0.52              |
| 10:C24:1297:HIS:NE2  | 10:C24:1372:ALA:CB   | 2.73                     | 0.52              |
| 11:A40:607:ARG:CZ    | 24:D32:914:PHE:CD1   | 2.89                     | 0.52              |
| 10:C:557:VAL:HG22    | 10:C:565:ARG:NE      | 2.23                     | 0.52              |
| 10:C:1553:VAL:HG23   | 10:C:1592:VAL:CG1    | 2.40                     | 0.52              |
| 10:C8:399:HIS:ND1    | 10:C8:400:PRO:HD2    | 2.24                     | 0.52              |
| 10:C8:959:GLU:HG2    | 10:C8:1139:ARG:HH21  | 1.75                     | 0.52              |
| 10:C8:1724:VAL:HG22  | 10:C8:1736:ILE:CD1   | 2.38                     | 0.52              |
| 11:A16:112:ALA:CB    | 18:B:1416:LYS:HZ3    | 2.22                     | 0.52              |
| 11:A16:448:GLU:OE1   | 17:F8:61:THR:HB      | 2.09                     | 0.52              |
| 11:A32:54:ASN:O      | 11:A32:59:GLN:NE2    | 2.43                     | 0.52              |
| 18:B:583:ARG:HD2     | 18:B:643:MET:SD      | 2.50                     | 0.52              |
| 18:B:686:LEU:HD11    | 18:B:790:ASP:CB      | 2.40                     | 0.52              |
| 18:B:1960:LEU:HD23   | 18:B:1961:TYR:CZ     | 2.45                     | 0.52              |
| 18:B8:12:TRP:CE2     | 18:B8:75:HIS:CD2     | 2.98                     | 0.52              |
| 18:B8:32:LEU:CD1     | 18:B8:163:ILE:CD1    | 2.83                     | 0.52              |
| 18:B8:313:ILE:HD13   | 18:B8:331:TRP:HB2    | 1.92                     | 0.52              |
| 21:H8:291:VAL:HG11   | 23:J8:657:GLU:HB3    | 1.91                     | 0.52              |
| 22:I8:193:GLU:OE1    | 22:I8:197:ARG:NH2    | 2.42                     | 0.52              |
| 23:J8:686:MET:HG2    | 23:J8:690:ASP:CB     | 2.39                     | 0.52              |
| 23:J24:686:MET:CE    | 23:J24:694:ARG:HH21  | 2.10                     | 0.52              |
| 22:I16:199:PHE:CG    | 23:J16:620:MET:CG    | 2.93                     | 0.52              |
| 24:D16:816:VAL:O     | 24:D16:824:LYS:HE3   | 2.09                     | 0.52              |
| 24:D16:1109:LEU:HD22 | 24:D16:1156:SER:HB2  | 1.91                     | 0.52              |
| 24:D16:1284:ILE:CD1  | 24:D16:1329:VAL:HG21 | 2.38                     | 0.52              |
| 24:D32:749:ARG:NH2   | 24:D40:397:ALA:HB3   | 2.25                     | 0.52              |
| 24:D40:1284:ILE:CD1  | 24:D40:1329:VAL:HG21 | 2.38                     | 0.52              |
| 10:C32:399:HIS:ND1   | 10:C32:400:PRO:HD2   | 2.24                     | 0.52              |
| 10:C32:619:LEU:CB    | 10:C32:620:PRO:CD    | 2.79                     | 0.52              |
| 10:C32:637:TYR:CZ    | 10:C32:642:GLU:OE2   | 2.61                     | 0.52              |
| 10:C32:898:GLN:NE2   | 10:C32:1138:GLU:CD   | 2.68                     | 0.52              |
| 10:C32:1076:TYR:O    | 10:C32:1077:ALA:C    | 2.49                     | 0.52              |
| 10:C32:1283:LEU:CD1  | 10:C32:1357:LEU:CD1  | 2.88                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A48:732:TYR:HE2  | 12:A48:738:VAL:HG11 | 1.74                     | 0.52              |
| 1:R:1428:VAL:HB     | 6:O:165:LYS:NZ      | 2.25                     | 0.52              |
| 1:R:1473:HIS:CD2    | 6:O:160:LEU:HB3     | 2.45                     | 0.52              |
| 2:M:166:THR:C       | 2:M:168:LEU:N       | 2.67                     | 0.52              |
| 2:M:417:ARG:CZ      | 8:L:298:PHE:O       | 2.58                     | 0.52              |
| 2:M:462:LEU:HD11    | 2:M:484:LEU:HD22    | 1.92                     | 0.52              |
| 2:M8:640:TYR:O      | 2:M8:644:TRP:CD1    | 2.63                     | 0.52              |
| 2:M8:816:ARG:NH2    | 2:M8:849:LEU:HB3    | 2.25                     | 0.52              |
| 2:M16:342:VAL:O     | 2:M16:344:GLN:N     | 2.43                     | 0.52              |
| 3:N16:97:HIS:HD2    | 3:N16:99:PHE:CE1    | 2.28                     | 0.52              |
| 5:P:569:VAL:O       | 5:P:643:PHE:CE2     | 2.63                     | 0.52              |
| 5:P8:582:GLU:HG2    | 5:P8:605:ARG:HG3    | 1.92                     | 0.52              |
| 9:K:879:CYS:HB3     | 9:K:900:TYR:CD2     | 2.45                     | 0.52              |
| 9:K:950:LYS:NZ      | 9:K:977:GLU:HB3     | 2.25                     | 0.52              |
| 9:K16:975:MET:HG2   | 9:K16:985:PHE:CD1   | 2.44                     | 0.52              |
| 10:C16:22:THR:HB    | 10:C16:23:PRO:HD2   | 1.92                     | 0.52              |
| 10:C16:736:ILE:HD11 | 10:C16:794:LYS:HZ2  | 1.74                     | 0.52              |
| 10:C16:1449:GLU:OE2 | 24:D8:1151:SER:CA   | 2.54                     | 0.52              |
| 10:C24:244:ASN:HD22 | 10:C24:263:LEU:HD11 | 1.75                     | 0.52              |
| 10:C24:557:VAL:HG22 | 10:C24:565:ARG:HE   | 1.74                     | 0.52              |
| 10:C24:557:VAL:HA   | 10:C24:565:ARG:HE   | 1.74                     | 0.52              |
| 11:A40:54:ASN:CB    | 11:A40:59:GLN:HE22  | 2.21                     | 0.52              |
| 12:A:109:HIS:CE1    | 10:C:1255:GLN:OE1   | 2.62                     | 0.52              |
| 14:W:198:LEU:HB3    | 14:W:400:ARG:HH12   | 1.75                     | 0.52              |
| 10:C:764:ILE:CD1    | 10:C:781:VAL:CG2    | 2.86                     | 0.52              |
| 10:C:1061:ASN:O     | 10:C:1063:PRO:HD3   | 2.10                     | 0.52              |
| 10:C8:792:PHE:HD1   | 10:C8:850:ARG:CZ    | 2.23                     | 0.52              |
| 10:C8:1250:ALA:CB   | 10:C8:1309:ARG:HH12 | 2.15                     | 0.52              |
| 11:A16:54:ASN:O     | 11:A16:59:GLN:NE2   | 2.43                     | 0.52              |
| 11:A16:489:PHE:CZ   | 17:F8:56:PRO:HA     | 2.45                     | 0.52              |
| 18:B:671:MET:HE1    | 18:B:733:VAL:HA     | 1.92                     | 0.52              |
| 18:B:1122:SER:C     | 18:B:1124:GLY:N     | 2.67                     | 0.52              |
| 18:B:1129:LYS:C     | 18:B:1131:THR:H     | 2.17                     | 0.52              |
| 18:B:1674:ASP:C     | 18:B:1676:VAL:N     | 2.68                     | 0.52              |
| 18:B8:496:LEU:HD22  | 18:B8:540:ILE:HD12  | 1.92                     | 0.52              |
| 18:B8:689:SER:C     | 18:B8:691:SER:H     | 2.16                     | 0.52              |
| 19:4:163:ALA:HB2    | 19:4:218:LEU:HD11   | 1.92                     | 0.52              |
| 19:4:230:ALA:HB2    | 19:4:260:LEU:HD11   | 1.92                     | 0.52              |
| 20:E:174:GLY:HA3    | 20:E:236:HIS:CE1    | 2.45                     | 0.52              |
| 19:48:251:ARG:HH21  | 19:48:254:LEU:CD2   | 2.19                     | 0.52              |
| 22:I24:131:ARG:CG   | 23:J24:557:ARG:CZ   | 2.64                     | 0.52              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 23:J16:686:MET:HG2   | 23:J16:690:ASP:HB2  | 1.91                     | 0.52              |
| 24:D:409:LEU:HD11    | 24:D16:746:ALA:N    | 2.15                     | 0.52              |
| 10:C32:931:PRO:HG2   | 10:C32:987:TYR:OH   | 2.10                     | 0.52              |
| 10:C32:1061:ASN:O    | 10:C32:1063:PRO:HD3 | 2.10                     | 0.52              |
| 10:C32:1271:PHE:HD1  | 10:C32:1273:GLY:H   | 1.54                     | 0.52              |
| 2:M:250:LEU:CD2      | 2:M:287:TYR:CD2     | 2.92                     | 0.52              |
| 1:R8:1379:GLN:HE22   | 1:R8:1416:TYR:HE1   | 1.56                     | 0.52              |
| 3:N8:97:HIS:HD2      | 3:N8:99:PHE:CE1     | 2.28                     | 0.52              |
| 1:R16:1442:THR:HG22  | 3:N16:13:ILE:HD11   | 1.91                     | 0.52              |
| 5:P:167:SER:CB       | 5:P:398:LYS:HE3     | 2.40                     | 0.52              |
| 7:Q:287:VAL:HG12     | 7:Q:307:THR:HG22    | 1.92                     | 0.52              |
| 5:P8:611:LEU:HG      | 5:P8:629:ARG:NE     | 2.24                     | 0.52              |
| 7:Q8:33:ARG:HH22     | 7:Q8:345:ASP:CB     | 2.23                     | 0.52              |
| 7:Q8:219:GLY:C       | 7:Q8:221:TRP:CD1    | 2.88                     | 0.52              |
| 5:P16:643:PHE:C      | 5:P16:646:PRO:HD2   | 2.35                     | 0.52              |
| 7:Q16:33:ARG:HH22    | 7:Q16:345:ASP:CB    | 2.23                     | 0.52              |
| 8:L16:1026:ARG:HD2   | 9:K16:1284:MET:HB3  | 1.87                     | 0.52              |
| 9:K8:1048:GLN:HG3    | 9:K8:1074:ARG:NH2   | 2.20                     | 0.52              |
| 10:C16:1283:LEU:HD23 | 10:C16:1287:MET:HE2 | 1.91                     | 0.52              |
| 10:C16:1821:VAL:CG1  | 11:A24:144:LYS:HE3  | 2.40                     | 0.52              |
| 10:C24:1280:VAL:CG2  | 10:C24:1731:HIS:ND1 | 2.72                     | 0.52              |
| 10:C24:1821:VAL:CG1  | 11:A40:144:LYS:HE3  | 2.40                     | 0.52              |
| 11:A40:10:TRP:CH2    | 21:H16:338:MET:HE3  | 2.45                     | 0.52              |
| 11:A40:107:GLN:NE2   | 21:H16:325:PRO:HA   | 2.25                     | 0.52              |
| 11:A40:785:HIS:CB    | 11:A40:793:ALA:HB2  | 2.39                     | 0.52              |
| 12:A:288:HIS:CE1     | 12:A:292:ILE:HD11   | 2.45                     | 0.52              |
| 12:A:794:THR:C       | 12:A:796:ASP:H      | 2.17                     | 0.52              |
| 10:C:1553:VAL:HG23   | 10:C:1592:VAL:HG12  | 1.91                     | 0.52              |
| 10:C8:286:ILE:HG21   | 10:C8:292:PHE:CE1   | 2.45                     | 0.52              |
| 10:C8:898:GLN:NE2    | 10:C8:1138:GLU:CD   | 2.59                     | 0.52              |
| 10:C8:1821:VAL:CG1   | 16:A8:144:LYS:HE3   | 2.40                     | 0.52              |
| 11:A16:121:GLN:HE22  | 18:B:1559:ALA:HB2   | 1.61                     | 0.52              |
| 11:A16:643:SER:O     | 11:A16:659:ARG:CD   | 2.58                     | 0.52              |
| 18:B:12:TRP:CE2      | 18:B:75:HIS:CD2     | 2.98                     | 0.52              |
| 18:B:277:GLU:OE2     | 18:B:393:VAL:HG22   | 2.09                     | 0.52              |
| 18:B8:686:LEU:HD11   | 18:B8:790:ASP:CB    | 2.40                     | 0.52              |
| 19:48:230:ALA:HB2    | 19:48:260:LEU:HD11  | 1.92                     | 0.52              |
| 21:H:258:MET:HG2     | 22:I:261:PHE:CD1    | 2.45                     | 0.52              |
| 22:I24:300:LEU:HD13  | 23:J24:689:LEU:CD2  | 2.40                     | 0.52              |
| 24:D16:22:ARG:HH21   | 24:D16:659:LEU:HD21 | 1.73                     | 0.52              |
| 10:C32:16:LEU:HD21   | 10:C32:139:ARG:NH1  | 2.24                     | 0.52              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C32:1002:LEU:CD2 | 10:C32:1012:ARG:CZ   | 2.79                     | 0.52              |
| 2:M:625:HIS:CD2     | 3:N:225:PRO:CA       | 2.93                     | 0.51              |
| 2:M:625:HIS:HE2     | 3:N:225:PRO:CB       | 2.23                     | 0.51              |
| 2:M:847:PHE:CE1     | 4:T:656:TRP:HB3      | 1.98                     | 0.51              |
| 1:R16:526:ASN:CA    | 1:R16:529:HIS:HE1    | 2.21                     | 0.51              |
| 5:P:398:LYS:HD2     | 5:P:426:MET:CE       | 2.40                     | 0.51              |
| 7:Q:30:ALA:HB1      | 10:C8:815:GLN:HE22   | 1.74                     | 0.51              |
| 7:Q:32:ASN:HB3      | 7:Q:34:PHE:CE2       | 2.45                     | 0.51              |
| 5:P8:207:HIS:CD2    | 5:P8:393:VAL:CG1     | 2.93                     | 0.51              |
| 5:P8:288:ARG:O      | 5:P8:299:CYS:HB3     | 2.08                     | 0.51              |
| 7:Q16:221:TRP:CD1   | 7:Q16:221:TRP:N      | 2.78                     | 0.51              |
| 8:L:346:TRP:CE3     | 8:L:346:TRP:C        | 2.88                     | 0.51              |
| 8:L8:614:GLU:CD     | 8:L8:649:LYS:NZ      | 2.68                     | 0.51              |
| 9:K:577:GLN:CD      | 9:K:625:ARG:HH11     | 2.18                     | 0.51              |
| 9:K:585:GLU:HA      | 9:K:622:VAL:HG13     | 1.91                     | 0.51              |
| 9:K:955:TYR:CD1     | 9:K:985:PHE:CD2      | 2.98                     | 0.51              |
| 9:K8:700:MET:HE3    | 9:K8:764:VAL:HA      | 1.92                     | 0.51              |
| 10:C16:168:ARG:HH12 | 10:C16:229:PRO:HA    | 1.70                     | 0.51              |
| 10:C16:1283:LEU:CD1 | 10:C16:1357:LEU:CD1  | 2.88                     | 0.51              |
| 11:A24:9:GLY:HA3    | 21:H8:339:GLN:HE22   | 1.74                     | 0.51              |
| 11:A24:643:SER:O    | 11:A24:659:ARG:CD    | 2.58                     | 0.51              |
| 10:C24:898:GLN:NE2  | 10:C24:1138:GLU:CD   | 2.68                     | 0.51              |
| 10:C24:1250:ALA:CB  | 10:C24:1309:ARG:HH12 | 2.15                     | 0.51              |
| 10:C24:1283:LEU:CD1 | 10:C24:1357:LEU:CD1  | 2.87                     | 0.51              |
| 11:A40:468:VAL:HG11 | 24:D32:1100:GLN:CB   | 2.40                     | 0.51              |
| 11:A40:501:PRO:CB   | 11:A40:524:GLU:OE1   | 2.58                     | 0.51              |
| 11:A40:643:SER:O    | 11:A40:659:ARG:CD    | 2.58                     | 0.51              |
| 13:V:776:LEU:HD13   | 14:W:664:ASN:OD1     | 2.10                     | 0.51              |
| 13:V:844:MET:HG3    | 10:C8:1502:ARG:CZ    | 2.39                     | 0.51              |
| 13:V:882:VAL:C      | 13:V:884:ASN:H       | 2.18                     | 0.51              |
| 10:C:878:ARG:NH2    | 10:C:885:VAL:CG2     | 2.69                     | 0.51              |
| 10:C:1271:PHE:CD1   | 10:C:1731:HIS:NE2    | 2.75                     | 0.51              |
| 10:C:1280:VAL:CG2   | 10:C:1731:HIS:ND1    | 2.72                     | 0.51              |
| 10:C8:394:SER:HB3   | 10:C8:458:VAL:CG2    | 2.37                     | 0.51              |
| 10:C8:925:GLU:OE1   | 10:C8:973:LEU:HD23   | 2.08                     | 0.51              |
| 10:C8:1760:GLU:OE2  | 16:A8:140:TRP:NE1    | 2.43                     | 0.51              |
| 11:A16:440:LEU:CG   | 11:A16:443:LEU:HD11  | 2.39                     | 0.51              |
| 11:A32:489:PHE:CZ   | 17:F24:56:PRO:HA     | 2.45                     | 0.51              |
| 11:A32:674:GLY:HA3  | 24:D32:1396:PRO:CG   | 2.38                     | 0.51              |
| 18:B:374:ILE:HG22   | 18:B:380:LEU:HD13    | 1.91                     | 0.51              |
| 18:B:1210:CYS:HG    | 18:B:1234:MET:CE     | 2.01                     | 0.51              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:1441:LEU:HA     | 18:B:1444:LEU:HD12   | 1.92                     | 0.51              |
| 18:B:1620:TRP:NE1    | 18:B:1624:LEU:HD11   | 2.26                     | 0.51              |
| 18:B:1799:VAL:C      | 18:B:1801:GLY:N      | 2.67                     | 0.51              |
| 18:B8:497:PHE:CE1    | 18:B8:512:VAL:HG11   | 2.44                     | 0.51              |
| 18:B8:1122:SER:C     | 18:B8:1124:GLY:N     | 2.67                     | 0.51              |
| 19:48:4:PHE:CD2      | 19:48:378:TYR:HE1    | 2.24                     | 0.51              |
| 24:D:409:LEU:HD21    | 24:D16:745:GLY:HA2   | 1.92                     | 0.51              |
| 10:C32:1094:LEU:HD21 | 10:C32:1203:MET:HB3  | 1.91                     | 0.51              |
| 10:C32:1250:ALA:CB   | 10:C32:1309:ARG:HH11 | 2.23                     | 0.51              |
| 10:C32:1283:LEU:HD23 | 10:C32:1287:MET:HE2  | 1.92                     | 0.51              |
| 1:R:1360:GLN:O       | 10:C:608:ASP:CG      | 2.54                     | 0.51              |
| 2:M:417:ARG:CG       | 8:L:346:TRP:CZ2      | 2.93                     | 0.51              |
| 2:M:847:PHE:CD1      | 4:T:656:TRP:CE3      | 2.59                     | 0.51              |
| 2:M:847:PHE:CD1      | 4:T:656:TRP:HE3      | 2.21                     | 0.51              |
| 3:N:158:TRP:HA       | 3:N:179:LEU:HD23     | 1.92                     | 0.51              |
| 1:R8:1124:TRP:HZ2    | 4:T8:669:PRO:CG      | 2.14                     | 0.51              |
| 2:M8:403:LEU:CD2     | 2:M8:425:ALA:HB3     | 2.40                     | 0.51              |
| 5:P16:167:SER:CB     | 5:P16:398:LYS:HE3    | 2.40                     | 0.51              |
| 6:O16:54:VAL:HG13    | 6:O16:85:TRP:CE2     | 2.45                     | 0.51              |
| 7:Q16:32:ASN:HB3     | 7:Q16:34:PHE:CE2     | 2.45                     | 0.51              |
| 7:Q16:295:SER:HB2    | 7:Q16:297:VAL:CG2    | 2.39                     | 0.51              |
| 7:Q16:297:VAL:HG12   | 7:Q16:298:SER:O      | 2.11                     | 0.51              |
| 8:L:1096:GLU:CG      | 9:K:998:GLN:HE21     | 2.23                     | 0.51              |
| 9:K8:577:GLN:CD      | 9:K8:625:ARG:HH11    | 2.18                     | 0.51              |
| 10:C16:26:ARG:HG2    | 10:C16:151:LEU:HD13  | 1.93                     | 0.51              |
| 10:C16:345:MET:HE1   | 10:C16:401:ILE:HD11  | 1.12                     | 0.51              |
| 10:C16:1074:LEU:HG   | 10:C16:1075:ASP:N    | 2.25                     | 0.51              |
| 10:C16:1553:VAL:HG23 | 10:C16:1592:VAL:CG1  | 2.40                     | 0.51              |
| 11:A24:489:PHE:CZ    | 17:F:56:PRO:HA       | 2.45                     | 0.51              |
| 11:A24:785:HIS:CB    | 11:A24:793:ALA:HB2   | 2.39                     | 0.51              |
| 10:C24:390:HIS:HD1   | 10:C24:452:LEU:CB    | 2.18                     | 0.51              |
| 10:C24:1553:VAL:HG23 | 10:C24:1592:VAL:CG1  | 2.40                     | 0.51              |
| 10:C24:1760:GLU:OE2  | 11:A40:140:TRP:NE1   | 2.43                     | 0.51              |
| 10:C:234:VAL:HG21    | 10:C:286:ILE:HD13    | 1.92                     | 0.51              |
| 10:C:1297:HIS:NE2    | 10:C:1372:ALA:CB     | 2.73                     | 0.51              |
| 10:C8:16:LEU:HD21    | 10:C8:139:ARG:NH1    | 2.24                     | 0.51              |
| 10:C8:26:ARG:HG2     | 10:C8:151:LEU:HD13   | 1.93                     | 0.51              |
| 10:C8:1280:VAL:CG2   | 10:C8:1731:HIS:ND1   | 2.72                     | 0.51              |
| 10:C8:1333:HIS:CE1   | 10:C8:1337:LEU:HD23  | 2.38                     | 0.51              |
| 11:A16:148:LEU:HD13  | 18:B:1956:ILE:CD1    | 2.37                     | 0.51              |
| 11:A16:151:LEU:O     | 18:B:1915:GLN:OE1    | 2.28                     | 0.51              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A16:288:HIS:CE1   | 11:A16:292:ILE:HD11  | 2.45                     | 0.51              |
| 11:A16:323:LEU:CD2   | 17:F8:74:ILE:HD12    | 2.36                     | 0.51              |
| 11:A32:676:TYR:CD2   | 24:D32:1395:SER:HB2  | 2.40                     | 0.51              |
| 18:B:495:THR:CG2     | 18:B:549:TRP:NE1     | 2.74                     | 0.51              |
| 18:B:1129:LYS:C      | 18:B:1131:THR:N      | 2.68                     | 0.51              |
| 18:B:1529:GLU:OE1    | 24:D16:1411:ASN:CB   | 2.58                     | 0.51              |
| 18:B8:1911:LEU:HB2   | 18:B8:1960:LEU:HD13  | 1.92                     | 0.51              |
| 19:48:175:TYR:CE2    | 20:E8:518:GLN:HA     | 2.45                     | 0.51              |
| 20:E8:332:LEU:O      | 20:E8:336:PHE:CD2    | 2.63                     | 0.51              |
| 21:H8:255:LEU:HD13   | 23:J8:655:GLU:OE2    | 2.01                     | 0.51              |
| 21:H16:322:LEU:HD22  | 22:I16:300:LEU:HG    | 1.89                     | 0.51              |
| 24:D:308:ASN:ND2     | 24:D16:753:ARG:HG3   | 2.24                     | 0.51              |
| 24:D24:1284:ILE:CD1  | 24:D24:1329:VAL:HG21 | 2.38                     | 0.51              |
| 10:C32:37:PHE:HB3    | 10:C32:38:PRO:HD3    | 1.91                     | 0.51              |
| 10:C32:792:PHE:HD1   | 10:C32:850:ARG:CZ    | 2.23                     | 0.51              |
| 10:C32:1553:VAL:HG23 | 10:C32:1592:VAL:CG1  | 2.40                     | 0.51              |
| 12:A48:288:HIS:CE1   | 12:A48:292:ILE:HD11  | 2.45                     | 0.51              |
| 2:M:346:VAL:C        | 2:M:348:GLU:H        | 2.18                     | 0.51              |
| 2:M:578:ARG:NH2      | 2:M:582:GLU:OE2      | 2.44                     | 0.51              |
| 2:M:625:HIS:ND1      | 3:N:165:GLY:HA2      | 2.24                     | 0.51              |
| 2:M:741:SER:OG       | 2:M:775:ARG:NH1      | 2.41                     | 0.51              |
| 1:R8:526:ASN:O       | 1:R8:529:HIS:HE1     | 1.93                     | 0.51              |
| 1:R8:982:GLU:CD      | 24:D40:1436:ARG:HE   | 2.17                     | 0.51              |
| 2:M8:342:VAL:O       | 2:M8:344:GLN:N       | 2.43                     | 0.51              |
| 2:M8:401:ARG:NH2     | 8:L8:381:GLU:OE2     | 2.43                     | 0.51              |
| 3:N8:116:ILE:CG2     | 3:N8:177:TYR:HE1     | 2.19                     | 0.51              |
| 7:Q:219:GLY:C        | 7:Q:221:TRP:CD1      | 2.88                     | 0.51              |
| 7:Q:297:VAL:HG12     | 7:Q:298:SER:O        | 2.10                     | 0.51              |
| 7:Q8:181:ALA:HB3     | 7:Q8:198:TYR:CE2     | 2.44                     | 0.51              |
| 6:O16:105:ASN:HD21   | 6:O16:134:ARG:HH22   | 1.57                     | 0.51              |
| 7:Q16:219:GLY:C      | 7:Q16:221:TRP:H      | 2.15                     | 0.51              |
| 7:Q16:287:VAL:HG12   | 7:Q16:307:THR:HG22   | 1.92                     | 0.51              |
| 9:K8:806:LEU:CD1     | 9:K8:874:VAL:HG11    | 2.39                     | 0.51              |
| 9:K8:950:LYS:NZ      | 9:K8:977:GLU:HB3     | 2.25                     | 0.51              |
| 9:K8:962:CYS:SG      | 9:K8:970:LEU:HD23    | 2.51                     | 0.51              |
| 10:C16:931:PRO:HG2   | 10:C16:987:TYR:OH    | 2.10                     | 0.51              |
| 10:C24:446:GLU:O     | 10:C24:448:LYS:HG3   | 2.10                     | 0.51              |
| 11:A40:54:ASN:O      | 11:A40:59:GLN:NE2    | 2.43                     | 0.51              |
| 12:A:322:ARG:HH11    | 12:A:351:PHE:HZ      | 1.57                     | 0.51              |
| 10:C:37:PHE:N        | 10:C:38:PRO:CD       | 2.74                     | 0.51              |
| 10:C:553:LEU:HD23    | 10:C:595:THR:HG23    | 1.91                     | 0.51              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C8:22:THR:HB     | 10:C8:23:PRO:HD2     | 1.92                     | 0.51              |
| 10:C8:234:VAL:HG21  | 10:C8:286:ILE:HD13   | 1.93                     | 0.51              |
| 10:C8:764:ILE:CD1   | 10:C8:781:VAL:CG2    | 2.86                     | 0.51              |
| 11:A16:665:GLU:OE2  | 24:D16:1462:PHE:CZ   | 2.63                     | 0.51              |
| 11:A32:501:PRO:CB   | 11:A32:524:GLU:OE1   | 2.58                     | 0.51              |
| 11:A32:643:SER:O    | 11:A32:659:ARG:CD    | 2.58                     | 0.51              |
| 18:B:7:VAL:HG21     | 18:B:99:ILE:HD11     | 1.92                     | 0.51              |
| 18:B:503:SER:H      | 18:B:504:PRO:CD      | 2.23                     | 0.51              |
| 18:B:603:PHE:CB     | 18:B:619:ARG:HH22    | 2.22                     | 0.51              |
| 18:B:643:MET:HE2    | 18:B:711:CYS:HB3     | 1.88                     | 0.51              |
| 18:B:1679:ARG:C     | 18:B:1681:GLN:N      | 2.68                     | 0.51              |
| 18:B8:1110:LEU:HD22 | 21:H24:326:GLY:CA    | 2.05                     | 0.51              |
| 18:B8:1112:LYS:CE   | 21:H24:327:SER:O     | 2.58                     | 0.51              |
| 18:B8:1548:LEU:CD1  | 18:B8:1564:PHE:HE2   | 2.22                     | 0.51              |
| 22:I:199:PHE:CG     | 23:J32:620:MET:CG    | 2.93                     | 0.51              |
| 22:I16:203:GLN:OE1  | 22:I16:209:TRP:CZ2   | 2.62                     | 0.51              |
| 22:I16:273:LEU:CD2  | 23:J16:658:LEU:HD21  | 2.41                     | 0.51              |
| 23:J16:623:GLU:CD   | 23:J16:626:ARG:HH21  | 2.08                     | 0.51              |
| 24:D24:1428:ASN:OD1 | 24:D32:968:ILE:HD11  | 2.09                     | 0.51              |
| 24:D40:816:VAL:O    | 24:D40:824:LYS:HE3   | 2.09                     | 0.51              |
| 10:C32:33:ILE:HG22  | 10:C32:158:LEU:HD22  | 1.92                     | 0.51              |
| 10:C32:446:GLU:O    | 10:C32:448:LYS:HG3   | 2.10                     | 0.51              |
| 1:R:1059:ILE:HG21   | 24:D:1448:TYR:OH     | 2.02                     | 0.51              |
| 2:M:182:PHE:CD1     | 2:M:183:MET:HG2      | 2.45                     | 0.51              |
| 2:M:640:TYR:O       | 2:M:644:TRP:CD1      | 2.63                     | 0.51              |
| 2:M8:182:PHE:CD1    | 2:M8:183:MET:HG2     | 2.45                     | 0.51              |
| 2:M8:627:TYR:CA     | 3:N8:167:LEU:HD12    | 2.39                     | 0.51              |
| 3:N8:200:MET:HE3    | 3:N8:203:PHE:HD2     | 1.74                     | 0.51              |
| 2:M16:339:GLU:OE2   | 4:T8:638:SER:C       | 2.54                     | 0.51              |
| 2:M16:773:VAL:CG1   | 2:M16:829:ALA:HA     | 2.41                     | 0.51              |
| 6:O:119:ARG:CG      | 6:O:181:GLU:O        | 2.58                     | 0.51              |
| 7:Q:295:SER:HB2     | 7:Q:297:VAL:CG2      | 2.39                     | 0.51              |
| 5:P8:10:GLY:HA2     | 5:P8:26:TYR:CZ       | 2.46                     | 0.51              |
| 6:O8:282:GLU:CB     | 6:O8:284:TRP:CZ2     | 2.93                     | 0.51              |
| 5:P16:207:HIS:CD2   | 5:P16:393:VAL:CG1    | 2.93                     | 0.51              |
| 5:P16:402:LEU:HD13  | 5:P16:433:LEU:CD1    | 2.40                     | 0.51              |
| 7:Q16:114:ASP:O     | 7:Q16:119:ALA:HA     | 2.10                     | 0.51              |
| 10:C16:637:TYR:CZ   | 10:C16:642:GLU:OE2   | 2.61                     | 0.51              |
| 10:C16:1553:VAL:CG2 | 10:C16:1592:VAL:HG12 | 2.41                     | 0.51              |
| 10:C16:1760:GLU:OE2 | 11:A24:140:TRP:NE1   | 2.43                     | 0.51              |
| 11:A24:307:GLY:CA   | 20:E:387:LEU:CD2     | 2.88                     | 0.51              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C24:26:ARG:HG2    | 10:C24:151:LEU:HD13 | 1.93                     | 0.51              |
| 10:C24:267:LEU:HB2   | 10:C24:316:ILE:CD1  | 2.41                     | 0.51              |
| 10:C24:470:HIS:CD2   | 10:C24:508:ILE:HD11 | 2.44                     | 0.51              |
| 10:C24:1637:PHE:CE1  | 11:A40:136:LEU:CD1  | 2.89                     | 0.51              |
| 12:A:641:ARG:C       | 12:A:685:ARG:NH2    | 2.69                     | 0.51              |
| 10:C8:1283:LEU:HD23  | 10:C8:1287:MET:HE2  | 1.91                     | 0.51              |
| 11:A32:10:TRP:CH2    | 21:H24:338:MET:HE3  | 2.45                     | 0.51              |
| 11:A32:151:LEU:O     | 18:B8:1915:GLN:OE1  | 2.28                     | 0.51              |
| 11:A32:257:GLN:CD    | 11:A32:263:ASP:CG   | 2.79                     | 0.51              |
| 11:A32:288:HIS:CE1   | 11:A32:292:ILE:HD11 | 2.45                     | 0.51              |
| 18:B:34:GLN:N        | 18:B:35:PRO:CD      | 2.72                     | 0.51              |
| 18:B:1142:PHE:CE2    | 18:B:1348:VAL:CG1   | 2.93                     | 0.51              |
| 18:B8:495:THR:CG2    | 18:B8:549:TRP:NE1   | 2.74                     | 0.51              |
| 18:B8:968:PHE:CG     | 18:B8:1040:MET:HE2  | 2.46                     | 0.51              |
| 18:B8:1439:LYS:CE    | 24:D32:1257:ASN:CG  | 2.82                     | 0.51              |
| 18:B8:1911:LEU:HA    | 18:B8:1960:LEU:CD1  | 2.40                     | 0.51              |
| 19:4:175:TYR:CE2     | 20:E:518:GLN:HA     | 2.45                     | 0.51              |
| 20:E:480:MET:HE2     | 20:E:493:TRP:CD2    | 2.46                     | 0.51              |
| 21:H8:258:MET:HG2    | 22:I8:261:PHE:CD1   | 2.45                     | 0.51              |
| 21:H8:366:MET:HE3    | 22:I8:332:MET:CE    | 2.32                     | 0.51              |
| 21:H24:151:LEU:HD12  | 21:H24:194:VAL:HG21 | 1.92                     | 0.51              |
| 21:H16:291:VAL:CG2   | 22:I16:273:LEU:HD21 | 2.41                     | 0.51              |
| 24:D:403:ARG:CA      | 24:D16:748:GLU:OE1  | 2.59                     | 0.51              |
| 10:C32:234:VAL:HG21  | 10:C32:286:ILE:HD13 | 1.93                     | 0.51              |
| 10:C32:244:ASN:HD22  | 10:C32:263:LEU:HD11 | 1.75                     | 0.51              |
| 1:R:1449:TRP:CH2     | 2:M:160:LEU:HG      | 2.46                     | 0.51              |
| 2:M:319:LYS:O        | 2:M:323:SER:OG      | 2.25                     | 0.51              |
| 1:R8:1075:LYS:HE2    | 5:P8:713:LEU:C      | 2.35                     | 0.51              |
| 2:M8:462:LEU:HD11    | 2:M8:484:LEU:HD22   | 1.92                     | 0.51              |
| 2:M8:844:VAL:CG2     | 4:T8:660:LEU:HD11   | 2.34                     | 0.51              |
| 2:M16:344:GLN:O      | 2:M16:345:ASP:C     | 2.45                     | 0.51              |
| 5:P8:96:VAL:HG13     | 5:P8:481:ILE:CD1    | 2.35                     | 0.51              |
| 5:P8:167:SER:CB      | 5:P8:398:LYS:HE3    | 2.40                     | 0.51              |
| 5:P8:425:TRP:HD1     | 5:P8:465:TYR:OH     | 1.94                     | 0.51              |
| 6:O8:43:SER:HA       | 7:Q8:45:ASP:OD2     | 2.10                     | 0.51              |
| 5:P16:10:GLY:HA2     | 5:P16:26:TYR:CZ     | 2.45                     | 0.51              |
| 9:K:700:MET:HE3      | 9:K:764:VAL:HA      | 1.92                     | 0.51              |
| 10:C16:37:PHE:HB3    | 10:C16:38:PRO:HD3   | 1.91                     | 0.51              |
| 10:C16:267:LEU:HB2   | 10:C16:316:ILE:CD1  | 2.41                     | 0.51              |
| 10:C16:446:GLU:O     | 10:C16:448:LYS:HG3  | 2.10                     | 0.51              |
| 10:C24:1164:VAL:HG13 | 10:C24:1167:PHE:CE2 | 2.46                     | 0.51              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 11:A40:56:ALA:HB1   | 11:A40:58:SER:OG     | 2.11                     | 0.51              |
| 10:C:267:LEU:HB2    | 10:C:316:ILE:CD1     | 2.41                     | 0.51              |
| 10:C8:139:ARG:HG3   | 10:C8:143:LEU:HD12   | 1.92                     | 0.51              |
| 10:C8:1002:LEU:CD1  | 10:C8:1019:ARG:NH1   | 2.64                     | 0.51              |
| 10:C8:1283:LEU:CD1  | 10:C8:1357:LEU:HD11  | 2.40                     | 0.51              |
| 10:C8:1624:LEU:HD22 | 10:C8:1628:SER:HB2   | 1.92                     | 0.51              |
| 18:B:496:LEU:HD22   | 18:B:540:ILE:HD12    | 1.92                     | 0.51              |
| 18:B:917:PHE:CE2    | 18:B:960:GLN:CD      | 2.85                     | 0.51              |
| 18:B8:374:ILE:HG22  | 18:B8:380:LEU:HD13   | 1.91                     | 0.51              |
| 18:B8:1161:LEU:HD21 | 18:B8:1164:GLU:OE2   | 2.11                     | 0.51              |
| 20:E:49:THR:HA      | 20:E:121:VAL:CG1     | 2.40                     | 0.51              |
| 19:48:57:ASN:C      | 19:48:59:GLY:H       | 2.19                     | 0.51              |
| 20:E8:480:MET:HE2   | 20:E8:493:TRP:CD2    | 2.46                     | 0.51              |
| 23:J32:718:GLN:HG3  | 23:J32:737:TRP:CH2   | 2.46                     | 0.51              |
| 21:H24:258:MET:HG2  | 22:I24:261:PHE:CD1   | 2.45                     | 0.51              |
| 21:H24:288:THR:OG1  | 23:J24:650:GLN:HG2   | 2.11                     | 0.51              |
| 21:H24:338:MET:HE3  | 23:J24:692:VAL:CG2   | 2.38                     | 0.51              |
| 22:I24:199:PHE:CG   | 23:J24:620:MET:CG    | 2.93                     | 0.51              |
| 24:D16:1452:LYS:HE2 | 24:D16:1456:GLU:OE1  | 2.11                     | 0.51              |
| 24:D24:275:LYS:HE3  | 24:D24:294:GLU:OE1   | 2.11                     | 0.51              |
| 10:C32:139:ARG:HG3  | 10:C32:143:LEU:HD12  | 1.93                     | 0.51              |
| 10:C32:705:TYR:O    | 10:C32:794:LYS:NZ    | 2.44                     | 0.51              |
| 10:C32:1553:VAL:CG2 | 10:C32:1592:VAL:HG12 | 2.41                     | 0.51              |
| 12:A48:288:HIS:CB   | 12:A48:354:ARG:NH1   | 2.71                     | 0.51              |
| 1:R:1139:ARG:HG3    | 1:R:1157:ARG:HH12    | 1.74                     | 0.51              |
| 1:R:1442:THR:HG22   | 3:N:13:ILE:HD11      | 1.91                     | 0.51              |
| 2:M:263:PHE:HE1     | 2:M:626:PRO:O        | 1.94                     | 0.51              |
| 2:M:627:TYR:CA      | 3:N:167:LEU:HD12     | 2.39                     | 0.51              |
| 1:R8:1165:MET:CE    | 5:P8:676:GLN:NE2     | 2.73                     | 0.51              |
| 1:R8:1175:TYR:CA    | 1:R8:1177:TRP:CZ3    | 2.79                     | 0.51              |
| 1:R16:1166:ASN:ND2  | 5:P16:672:LEU:CD2    | 2.65                     | 0.51              |
| 1:R16:1449:TRP:CH2  | 2:M16:160:LEU:HG     | 2.46                     | 0.51              |
| 7:Q:33:ARG:HH22     | 7:Q:345:ASP:CB       | 2.23                     | 0.51              |
| 7:Q:221:TRP:CD1     | 7:Q:221:TRP:N        | 2.78                     | 0.51              |
| 7:Q8:32:ASN:HB3     | 7:Q8:34:PHE:CE2      | 2.45                     | 0.51              |
| 7:Q8:287:VAL:HG12   | 7:Q8:307:THR:HG22    | 1.92                     | 0.51              |
| 7:Q8:297:VAL:HG12   | 7:Q8:298:SER:O       | 2.10                     | 0.51              |
| 9:K8:1085:TYR:CE1   | 9:K8:1093:SER:HA     | 2.09                     | 0.51              |
| 10:C16:234:VAL:HG21 | 10:C16:286:ILE:HD13  | 1.92                     | 0.51              |
| 11:A24:560:MET:HE2  | 11:A24:615:GLN:NE2   | 1.97                     | 0.51              |
| 10:C24:37:PHE:HB3   | 10:C24:38:PRO:HD3    | 1.91                     | 0.51              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C24:1283:LEU:HD23 | 10:C24:1287:MET:HE2 | 1.92                     | 0.51              |
| 11:A40:54:ASN:O      | 11:A40:59:GLN:CD    | 2.54                     | 0.51              |
| 14:W:713:GLU:O       | 15:J:647:MET:HE1    | 2.10                     | 0.51              |
| 10:C:35:ASN:CG       | 24:D:1148:LEU:HD11  | 2.36                     | 0.51              |
| 10:C8:267:LEU:HB2    | 10:C8:316:ILE:CD1   | 2.41                     | 0.51              |
| 10:C8:1424:GLN:HE21  | 10:C8:1478:VAL:HG13 | 1.72                     | 0.51              |
| 11:A16:10:TRP:CH2    | 21:H:338:MET:HE3    | 2.45                     | 0.51              |
| 11:A32:785:HIS:ND1   | 11:A32:793:ALA:HB2  | 2.26                     | 0.51              |
| 18:B:968:PHE:CG      | 18:B:1040:MET:HE2   | 2.46                     | 0.51              |
| 18:B:1548:LEU:CD1    | 18:B:1564:PHE:HE2   | 2.22                     | 0.51              |
| 18:B8:491:VAL:HG12   | 18:B8:552:SER:HA    | 1.92                     | 0.51              |
| 18:B8:583:ARG:HD2    | 18:B8:643:MET:SD    | 2.50                     | 0.51              |
| 18:B8:917:PHE:CE2    | 18:B8:960:GLN:CD    | 2.85                     | 0.51              |
| 19:4:305:TRP:CE2     | 19:4:312:ILE:HD12   | 2.46                     | 0.51              |
| 20:E:333:ASP:O       | 20:E:337:THR:OG1    | 2.21                     | 0.51              |
| 19:48:361:ASP:OD2    | 19:48:363:SER:OG    | 2.26                     | 0.51              |
| 19:48:362:ALA:N      | 19:48:417:ASP:OD2   | 2.34                     | 0.51              |
| 22:I:300:LEU:HD13    | 23:J32:689:LEU:CD2  | 2.40                     | 0.51              |
| 21:H8:151:LEU:HD12   | 21:H8:194:VAL:HG21  | 1.92                     | 0.51              |
| 22:I24:203:GLN:OE1   | 22:I24:209:TRP:HZ2  | 1.94                     | 0.51              |
| 10:C32:26:ARG:HG2    | 10:C32:151:LEU:HD13 | 1.93                     | 0.51              |
| 12:A48:257:GLN:CD    | 12:A48:263:ASP:OD1  | 2.51                     | 0.51              |
| 12:A48:785:HIS:ND1   | 12:A48:793:ALA:HB2  | 2.26                     | 0.51              |
| 2:M8:263:PHE:HE1     | 2:M8:626:PRO:O      | 1.94                     | 0.51              |
| 2:M8:578:ARG:NH2     | 2:M8:582:GLU:OE2    | 2.44                     | 0.51              |
| 2:M8:627:TYR:HB3     | 3:N8:167:LEU:CG     | 2.40                     | 0.51              |
| 5:P:5:SER:O          | 5:P:7:GLU:N         | 2.44                     | 0.51              |
| 5:P:10:GLY:HA2       | 5:P:26:TYR:CZ       | 2.46                     | 0.51              |
| 5:P:207:HIS:CD2      | 5:P:393:VAL:CG1     | 2.93                     | 0.51              |
| 6:O8:179:LYS:O       | 6:O8:180:GLY:C      | 2.49                     | 0.51              |
| 6:O8:201:SER:OG      | 6:O8:232:LEU:HD21   | 2.09                     | 0.51              |
| 5:P16:12:GLU:HG3     | 5:P16:78:GLY:N      | 2.26                     | 0.51              |
| 5:P16:193:VAL:HG21   | 5:P16:368:LEU:HD21  | 1.92                     | 0.51              |
| 5:P16:425:TRP:HD1    | 5:P16:465:TYR:OH    | 1.94                     | 0.51              |
| 9:K:751:LEU:CD2      | 9:K:754:ARG:NH1     | 2.60                     | 0.51              |
| 10:C16:557:VAL:HG22  | 10:C16:565:ARG:HE   | 1.74                     | 0.51              |
| 10:C16:898:GLN:NE2   | 10:C16:1138:GLU:CD  | 2.68                     | 0.51              |
| 10:C16:1050:HIS:CE1  | 10:C16:1086:LYS:HZ1 | 2.20                     | 0.51              |
| 11:A24:54:ASN:O      | 11:A24:59:GLN:NE2   | 2.43                     | 0.51              |
| 11:A24:54:ASN:CB     | 11:A24:59:GLN:HE22  | 2.21                     | 0.51              |
| 11:A24:501:PRO:CB    | 11:A24:524:GLU:OE1  | 2.58                     | 0.51              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:248:LEU:HD11 | 10:C24:260:THR:OG1   | 2.11                     | 0.51              |
| 10:C24:1547:LYS:HE2 | 24:D24:1405:GLY:N    | 2.24                     | 0.51              |
| 10:C24:1553:VAL:CG2 | 10:C24:1592:VAL:HG12 | 2.41                     | 0.51              |
| 11:A40:9:GLY:HA3    | 21:H16:339:GLN:HE22  | 1.74                     | 0.51              |
| 11:A40:785:HIS:ND1  | 11:A40:793:ALA:HB2   | 2.26                     | 0.51              |
| 14:W:711:ARG:HD2    | 10:C8:1609:ASP:CG    | 2.21                     | 0.51              |
| 10:C8:1129:VAL:HG12 | 10:C8:1130:SER:H     | 1.75                     | 0.51              |
| 11:A16:56:ALA:HB1   | 11:A16:58:SER:OG     | 2.11                     | 0.51              |
| 11:A32:400:CYS:SG   | 11:A32:423:TYR:HB3   | 2.51                     | 0.51              |
| 11:A32:448:GLU:OE2  | 17:F24:61:THR:HA     | 2.11                     | 0.51              |
| 18:B:7:VAL:HG11     | 18:B:99:ILE:CD1      | 2.41                     | 0.51              |
| 18:B:112:GLU:CD     | 18:B:130:MET:HE1     | 2.35                     | 0.51              |
| 18:B:693:SER:C      | 18:B:695:LYS:H       | 2.19                     | 0.51              |
| 18:B:771:MET:HE3    | 18:B:840:VAL:CG2     | 2.41                     | 0.51              |
| 18:B:1424:LEU:CD2   | 18:B:1490:ILE:HD12   | 2.40                     | 0.51              |
| 18:B8:112:GLU:CD    | 18:B8:130:MET:HE1    | 2.34                     | 0.51              |
| 18:B8:907:SER:C     | 18:B8:909:LEU:H      | 2.18                     | 0.51              |
| 18:B8:1139:LYS:CB   | 18:B8:1365:ARG:HH11  | 2.23                     | 0.51              |
| 18:B8:1590:LEU:HD22 | 18:B8:1620:TRP:HE3   | 1.76                     | 0.51              |
| 19:48:185:GLY:O     | 19:48:187:SER:N      | 2.41                     | 0.51              |
| 20:E8:345:LEU:HD21  | 24:D40:123:ALA:HB3   | 1.85                     | 0.51              |
| 20:E8:433:LYS:C     | 20:E8:435:ALA:N      | 2.60                     | 0.51              |
| 20:E8:447:ILE:CG2   | 20:E8:451:ILE:HG21   | 2.32                     | 0.51              |
| 21:H:151:LEU:HD12   | 21:H:194:VAL:HG21    | 1.92                     | 0.51              |
| 21:H8:288:THR:OG1   | 23:J8:650:GLN:HG2    | 2.11                     | 0.51              |
| 22:I8:273:LEU:CD2   | 23:J8:658:LEU:HD21   | 2.41                     | 0.51              |
| 23:J8:718:GLN:HG3   | 23:J8:737:TRP:CH2    | 2.46                     | 0.51              |
| 21:H24:291:VAL:CG2  | 22:I24:273:LEU:HD21  | 2.41                     | 0.51              |
| 21:H24:322:LEU:CG   | 22:I24:300:LEU:HD11  | 2.39                     | 0.51              |
| 24:D16:275:LYS:HE3  | 24:D16:294:GLU:OE1   | 2.11                     | 0.51              |
| 24:D32:275:LYS:HE3  | 24:D32:294:GLU:OE1   | 2.11                     | 0.51              |
| 10:C32:764:ILE:CD1  | 10:C32:781:VAL:CG2   | 2.86                     | 0.51              |
| 12:A48:400:CYS:SG   | 12:A48:423:TYR:HB3   | 2.51                     | 0.51              |
| 1:R:526:ASN:O       | 1:R:529:HIS:HE1      | 1.93                     | 0.51              |
| 2:M8:741:SER:OG     | 2:M8:775:ARG:NH1     | 2.41                     | 0.51              |
| 1:R16:526:ASN:O     | 1:R16:529:HIS:HE1    | 1.93                     | 0.51              |
| 2:M16:182:PHE:CD1   | 2:M16:183:MET:HG2    | 2.45                     | 0.51              |
| 7:Q:88:ASN:O        | 7:Q:89:GLY:O         | 2.29                     | 0.51              |
| 7:Q8:88:ASN:O       | 7:Q8:89:GLY:O        | 2.29                     | 0.51              |
| 9:K:788:LEU:HD22    | 9:K:856:ILE:CD1      | 2.19                     | 0.51              |
| 9:K:798:LEU:HB2     | 9:K:842:ILE:HD11     | 1.93                     | 0.51              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 9:K:962:CYS:SG       | 9:K:970:LEU:HD23    | 2.51                     | 0.51              |
| 10:C16:1548:ILE:HD12 | 24:D8:1407:PHE:CZ   | 2.16                     | 0.51              |
| 11:A24:54:ASN:O      | 11:A24:59:GLN:CD    | 2.54                     | 0.51              |
| 11:A24:448:GLU:OE2   | 17:F:61:THR:HA      | 2.11                     | 0.51              |
| 10:C24:637:TYR:CZ    | 10:C24:642:GLU:OE2  | 2.61                     | 0.51              |
| 11:A40:400:CYS:SG    | 11:A40:423:TYR:HB3  | 2.51                     | 0.51              |
| 11:A40:707:LEU:CD1   | 11:A40:767:ARG:HH22 | 2.17                     | 0.51              |
| 12:A:144:LYS:HE3     | 10:C:1821:VAL:CG1   | 2.40                     | 0.51              |
| 12:A:257:GLN:CD      | 12:A:263:ASP:CG     | 2.78                     | 0.51              |
| 12:A:288:HIS:CB      | 12:A:354:ARG:NH1    | 2.71                     | 0.51              |
| 12:A:362:ARG:CD      | 12:A:366:ARG:CZ     | 2.87                     | 0.51              |
| 14:W:714:LEU:O       | 10:C8:1568:ARG:CZ   | 2.58                     | 0.51              |
| 10:C:154:ASP:OD1     | 24:D:1403:LEU:HD21  | 2.11                     | 0.51              |
| 11:A16:362:ARG:CD    | 11:A16:366:ARG:CZ   | 2.87                     | 0.51              |
| 11:A32:56:ALA:HB1    | 11:A32:58:SER:OG    | 2.11                     | 0.51              |
| 11:A32:159:LYS:NZ    | 18:B8:1918:ARG:CG   | 2.74                     | 0.51              |
| 18:B:907:SER:C       | 18:B:909:LEU:H      | 2.18                     | 0.51              |
| 18:B8:603:PHE:CB     | 18:B8:619:ARG:HH22  | 2.22                     | 0.51              |
| 18:B8:693:SER:C      | 18:B8:695:LYS:H     | 2.19                     | 0.51              |
| 18:B8:1652:PHE:CZ    | 18:B8:1700:LEU:HD12 | 2.46                     | 0.51              |
| 18:B8:1774:TRP:CE3   | 18:B8:1823:ILE:HD13 | 2.46                     | 0.51              |
| 20:E8:432:ILE:CD1    | 24:D40:72:GLU:OE1   | 2.48                     | 0.51              |
| 24:D:405:GLN:NE2     | 24:D16:10:ARG:CZ    | 2.74                     | 0.51              |
| 24:D40:274:MET:CE    | 24:D40:321:SER:HB2  | 2.40                     | 0.51              |
| 10:C32:664:ASN:CA    | 10:C32:667:ILE:HG13 | 2.39                     | 0.51              |
| 12:A48:643:SER:O     | 12:A48:659:ARG:CD   | 2.58                     | 0.51              |
| 12:A48:785:HIS:CB    | 12:A48:793:ALA:HB2  | 2.39                     | 0.51              |
| 2:M:217:ILE:CD1      | 3:N:8:THR:CG2       | 2.89                     | 0.51              |
| 2:M:342:VAL:O        | 2:M:344:GLN:N       | 2.43                     | 0.51              |
| 2:M8:217:ILE:CD1     | 3:N8:8:THR:CG2      | 2.89                     | 0.51              |
| 2:M16:166:THR:C      | 2:M16:168:LEU:N     | 2.67                     | 0.51              |
| 2:M16:540:TYR:HD1    | 2:M16:555:LEU:HD22  | 1.30                     | 0.51              |
| 5:P16:214:LEU:HD21   | 5:P16:236:VAL:CG1   | 2.39                     | 0.51              |
| 5:P16:607:PHE:HB3    | 5:P16:629:ARG:CD    | 2.41                     | 0.51              |
| 9:K:751:LEU:HD21     | 9:K:754:ARG:HH11    | 1.68                     | 0.51              |
| 9:K:1048:GLN:CD      | 9:K:1128:ARG:CG     | 2.79                     | 0.51              |
| 9:K8:923:ILE:CG2     | 9:K8:929:ARG:NH2    | 2.72                     | 0.51              |
| 10:C16:33:ILE:HG22   | 10:C16:158:LEU:HD22 | 1.92                     | 0.51              |
| 10:C16:37:PHE:N      | 10:C16:38:PRO:CD    | 2.74                     | 0.51              |
| 10:C16:244:ASN:HD22  | 10:C16:263:LEU:HD11 | 1.75                     | 0.51              |
| 10:C16:962:PHE:HE2   | 10:C16:997:ILE:CD1  | 2.16                     | 0.51              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:1164:VAL:HG13 | 10:C16:1167:PHE:CE2 | 2.46                     | 0.51              |
| 11:A40:288:HIS:CE1   | 11:A40:292:ILE:HD11 | 2.45                     | 0.51              |
| 14:W:177:HIS:CD2     | 14:W:254:PRO:HB3    | 2.46                     | 0.51              |
| 10:C8:33:ILE:HG22    | 10:C8:158:LEU:HD22  | 1.93                     | 0.51              |
| 10:C8:278:ARG:NH1    | 10:C8:287:SER:CB    | 2.62                     | 0.51              |
| 10:C8:861:ILE:HG22   | 10:C8:861:ILE:O     | 2.10                     | 0.51              |
| 11:A16:501:PRO:CB    | 11:A16:524:GLU:OE1  | 2.58                     | 0.51              |
| 18:B8:1745:HIS:C     | 18:B8:1747:SER:H    | 2.19                     | 0.51              |
| 18:B8:1960:LEU:HD23  | 18:B8:1961:TYR:CZ   | 2.45                     | 0.51              |
| 19:4:4:PHE:CD2       | 19:4:378:TYR:HE1    | 2.24                     | 0.51              |
| 20:E:332:LEU:O       | 20:E:336:PHE:HD2    | 1.93                     | 0.51              |
| 20:E8:32:PHE:O       | 20:E8:36:PHE:HD2    | 1.92                     | 0.51              |
| 22:I8:300:LEU:HD13   | 23:J8:689:LEU:CD2   | 2.40                     | 0.51              |
| 21:H24:284:LEU:HD21  | 23:J24:650:GLN:HB3  | 1.92                     | 0.51              |
| 23:J24:718:GLN:HG3   | 23:J24:737:TRP:CH2  | 2.46                     | 0.51              |
| 24:D8:275:LYS:CE     | 24:D8:294:GLU:CD    | 2.84                     | 0.51              |
| 10:C32:663:ILE:CG2   | 10:C32:667:ILE:CG2  | 2.88                     | 0.51              |
| 10:C32:861:ILE:HG22  | 10:C32:861:ILE:O    | 2.11                     | 0.51              |
| 10:C32:1290:HIS:CB   | 10:C32:1334:MET:CE  | 2.72                     | 0.51              |
| 12:A48:403:MET:HA    | 12:A48:406:MET:HE3  | 1.93                     | 0.51              |
| 12:A48:501:PRO:CB    | 12:A48:524:GLU:OE1  | 2.58                     | 0.51              |
| 1:R:1328:LYS:CE      | 10:C:1177:ARG:NE    | 2.68                     | 0.51              |
| 1:R:1473:HIS:HD2     | 6:O:160:LEU:HD22    | 1.71                     | 0.51              |
| 2:M:519:TYR:O        | 2:M:523:GLY:HA3     | 2.11                     | 0.51              |
| 2:M:738:ILE:CD1      | 2:M:779:SER:CB      | 2.89                     | 0.51              |
| 1:R8:1182:PRO:C      | 1:R8:1184:GLU:N     | 2.68                     | 0.51              |
| 1:R8:1449:TRP:CH2    | 2:M8:160:LEU:HG     | 2.46                     | 0.51              |
| 2:M16:231:ARG:CG     | 2:M16:299:GLY:O     | 2.52                     | 0.51              |
| 2:M16:278:VAL:HG13   | 2:M16:326:GLN:HG3   | 1.91                     | 0.51              |
| 5:P:569:VAL:O        | 5:P:643:PHE:HE2     | 1.94                     | 0.51              |
| 5:P8:154:ASP:OD1     | 5:P8:155:PRO:HD2    | 2.11                     | 0.51              |
| 5:P16:101:LEU:HD23   | 5:P16:133:TYR:CE1   | 2.30                     | 0.51              |
| 9:K:959:TRP:CD2      | 9:K:992:GLN:HG3     | 2.46                     | 0.51              |
| 9:K8:879:CYS:HB3     | 9:K8:900:TYR:CD2    | 2.45                     | 0.51              |
| 9:K16:638:TRP:CZ3    | 9:K16:648:ALA:HB1   | 2.46                     | 0.51              |
| 10:C24:37:PHE:N      | 10:C24:38:PRO:CD    | 2.73                     | 0.51              |
| 10:C24:861:ILE:HG22  | 10:C24:861:ILE:O    | 2.10                     | 0.51              |
| 12:A:501:PRO:CB      | 12:A:524:GLU:OE1    | 2.58                     | 0.51              |
| 13:V:739:ARG:O       | 13:V:743:THR:OG1    | 2.29                     | 0.51              |
| 10:C:1033:GLY:CA     | 10:C:1218:ARG:NH2   | 2.74                     | 0.51              |
| 10:C8:244:ASN:HD22   | 10:C8:263:LEU:HD11  | 1.75                     | 0.51              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C8:1164:VAL:HG13  | 10:C8:1167:PHE:CE2  | 2.46                     | 0.51              |
| 10:C8:1297:HIS:NE2   | 10:C8:1372:ALA:CB   | 2.73                     | 0.51              |
| 10:C8:1637:PHE:CE1   | 16:A8:136:LEU:CD1   | 2.90                     | 0.51              |
| 11:A16:448:GLU:OE2   | 17:F8:61:THR:HA     | 2.11                     | 0.51              |
| 11:A16:785:HIS:CB    | 11:A16:793:ALA:HB2  | 2.39                     | 0.51              |
| 11:A32:362:ARG:CD    | 11:A32:366:ARG:CZ   | 2.87                     | 0.51              |
| 11:A32:706:SER:OG    | 24:D32:1398:ARG:HB3 | 2.11                     | 0.51              |
| 18:B:1739:LEU:HD22   | 18:B:1777:LEU:CD2   | 2.40                     | 0.51              |
| 18:B8:1620:TRP:NE1   | 18:B8:1624:LEU:HD11 | 2.26                     | 0.51              |
| 18:B8:1739:LEU:HD22  | 18:B8:1777:LEU:CD2  | 2.40                     | 0.51              |
| 20:E:358:GLY:C       | 20:E:454:MET:SD     | 2.94                     | 0.51              |
| 20:E8:39:SER:O       | 20:E8:39:SER:OG     | 2.27                     | 0.51              |
| 21:H8:321:SER:HB3    | 21:H8:323:TYR:HE1   | 1.72                     | 0.51              |
| 21:H8:322:LEU:CG     | 22:I8:300:LEU:HD11  | 2.39                     | 0.51              |
| 24:D:274:MET:CE      | 24:D:321:SER:HB2    | 2.40                     | 0.51              |
| 24:D40:865:VAL:CG2   | 24:D40:932:ARG:HH12 | 2.24                     | 0.51              |
| 24:D40:1452:LYS:HE2  | 24:D40:1456:GLU:OE1 | 2.11                     | 0.51              |
| 10:C32:22:THR:HB     | 10:C32:23:PRO:HD2   | 1.92                     | 0.51              |
| 10:C32:1821:VAL:CG1  | 12:A48:144:LYS:HE3  | 2.40                     | 0.51              |
| 12:A48:257:GLN:CD    | 12:A48:263:ASP:CG   | 2.78                     | 0.51              |
| 1:R:979:GLN:HB2      | 24:D:1438:ALA:HB3   | 1.90                     | 0.50              |
| 1:R:1334:GLU:HG2     | 10:C:1170:VAL:H     | 1.76                     | 0.50              |
| 1:R8:982:GLU:HG3     | 24:D40:1436:ARG:NE  | 2.26                     | 0.50              |
| 2:M8:166:THR:C       | 2:M8:168:LEU:H      | 2.19                     | 0.50              |
| 2:M8:310:HIS:HA      | 2:M8:313:MET:CE     | 2.41                     | 0.50              |
| 2:M16:263:PHE:HE1    | 2:M16:626:PRO:O     | 1.94                     | 0.50              |
| 2:M16:339:GLU:O      | 2:M16:341:ASP:N     | 2.44                     | 0.50              |
| 2:M16:420:CYS:CB     | 8:L16:391:TRP:CH2   | 2.93                     | 0.50              |
| 2:M16:462:LEU:HD11   | 2:M16:484:LEU:HD22  | 1.92                     | 0.50              |
| 5:P:154:ASP:OD1      | 5:P:155:PRO:HD2     | 2.11                     | 0.50              |
| 5:P:214:LEU:HD21     | 5:P:236:VAL:CG1     | 2.39                     | 0.50              |
| 5:P:241:LEU:O        | 5:P:369:TYR:OH      | 2.18                     | 0.50              |
| 7:Q8:52:GLN:OE1      | 7:Q8:68:ILE:HG21    | 2.11                     | 0.50              |
| 9:K:1007:GLU:OE1     | 9:K:1031:LEU:HD21   | 2.11                     | 0.50              |
| 9:K:1122:ALA:HB1     | 9:K:1127:PHE:HZ     | 1.77                     | 0.50              |
| 9:K8:1133:ILE:CG2    | 9:K8:1166:LEU:HD23  | 2.39                     | 0.50              |
| 10:C16:248:LEU:HD11  | 10:C16:260:THR:OG1  | 2.11                     | 0.50              |
| 10:C16:265:PHE:HE1   | 10:C16:389:LEU:HD12 | 1.76                     | 0.50              |
| 10:C16:1129:VAL:HG12 | 10:C16:1130:SER:H   | 1.75                     | 0.50              |
| 11:A24:56:ALA:HB1    | 11:A24:58:SER:OG    | 2.11                     | 0.50              |
| 11:A24:257:GLN:CD    | 11:A24:263:ASP:CG   | 2.79                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A24:381:TRP:CD1   | 11:A24:386:GLY:HA2   | 2.46                     | 0.50              |
| 10:C24:699:HIS:O     | 10:C24:703:SER:OG    | 2.23                     | 0.50              |
| 10:C24:792:PHE:HD1   | 10:C24:850:ARG:CZ    | 2.23                     | 0.50              |
| 11:A40:448:GLU:OE2   | 17:F16:61:THR:HA     | 2.11                     | 0.50              |
| 12:A:136:LEU:CD1     | 10:C:1637:PHE:CE1    | 2.90                     | 0.50              |
| 12:A:381:TRP:CD1     | 12:A:386:GLY:HA2     | 2.46                     | 0.50              |
| 12:A:440:LEU:CG      | 12:A:443:LEU:HD11    | 2.39                     | 0.50              |
| 12:A:785:HIS:ND1     | 12:A:793:ALA:HB2     | 2.26                     | 0.50              |
| 10:C:139:ARG:HG3     | 10:C:143:LEU:HD12    | 1.93                     | 0.50              |
| 10:C:244:ASN:HD22    | 10:C:263:LEU:HD11    | 1.75                     | 0.50              |
| 10:C:452:LEU:HD12    | 10:C:453:LEU:CA      | 2.41                     | 0.50              |
| 10:C:1154:TRP:CZ2    | 10:C:1158:HIS:CE1    | 2.99                     | 0.50              |
| 10:C8:556:VAL:O      | 10:C8:565:ARG:NH2    | 2.44                     | 0.50              |
| 10:C8:663:ILE:CG2    | 10:C8:667:ILE:CG2    | 2.90                     | 0.50              |
| 10:C8:736:ILE:HD11   | 10:C8:794:LYS:HZ2    | 1.76                     | 0.50              |
| 11:A16:159:LYS:NZ    | 18:B:1918:ARG:CG     | 2.74                     | 0.50              |
| 11:A16:785:HIS:ND1   | 11:A16:793:ALA:HB2   | 2.26                     | 0.50              |
| 18:B:1652:PHE:CZ     | 18:B:1700:LEU:HD12   | 2.46                     | 0.50              |
| 18:B8:1424:LEU:CD2   | 18:B8:1490:ILE:HD12  | 2.40                     | 0.50              |
| 18:B8:1685:THR:HG22  | 18:B8:1689:TYR:CD1   | 2.46                     | 0.50              |
| 20:E8:358:GLY:C      | 20:E8:454:MET:SD     | 2.94                     | 0.50              |
| 24:D:400:VAL:CG2     | 24:D16:751:MET:HB2   | 2.41                     | 0.50              |
| 10:C32:267:LEU:HB2   | 10:C32:316:ILE:CD1   | 2.41                     | 0.50              |
| 10:C32:1132:SER:OG   | 10:C32:1134:TYR:O    | 2.29                     | 0.50              |
| 10:C32:1352:GLN:NE2  | 10:C32:1357:LEU:CD1  | 2.74                     | 0.50              |
| 1:R:1078:SER:C       | 5:P:713:LEU:HD21     | 2.36                     | 0.50              |
| 2:M8:773:VAL:CG1     | 2:M8:829:ALA:HA      | 2.41                     | 0.50              |
| 1:R16:1194:ARG:O     | 1:R16:1195:ARG:C     | 2.52                     | 0.50              |
| 2:M16:217:ILE:CD1    | 3:N16:8:THR:CG2      | 2.89                     | 0.50              |
| 2:M16:844:VAL:CG2    | 4:T16:660:LEU:HD11   | 2.34                     | 0.50              |
| 5:P:12:GLU:HG3       | 5:P:78:GLY:N         | 2.26                     | 0.50              |
| 5:P:16:PHE:HD1       | 6:O:311:LEU:HD12     | 1.76                     | 0.50              |
| 5:P:425:TRP:HD1      | 5:P:465:TYR:OH       | 1.94                     | 0.50              |
| 7:Q:78:SER:OG        | 7:Q:103:THR:HB       | 2.12                     | 0.50              |
| 7:Q:331:CYS:HB3      | 7:Q:352:TRP:CE2      | 2.46                     | 0.50              |
| 5:P8:12:GLU:HG3      | 5:P8:78:GLY:N        | 2.26                     | 0.50              |
| 6:O8:105:ASN:ND2     | 6:O8:134:ARG:NH2     | 2.59                     | 0.50              |
| 8:L8:175:ARG:NH1     | 12:A48:134:LYS:CD    | 2.71                     | 0.50              |
| 9:K:1064:PRO:C       | 9:K:1066:ASP:N       | 2.68                     | 0.50              |
| 10:C16:1126:ASP:CG   | 24:D8:1069:GLY:CA    | 2.81                     | 0.50              |
| 10:C16:1211:VAL:HG11 | 10:C16:1232:ILE:HG21 | 1.94                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1601:TYR:C    | 10:C24:1665:THR:HG21 | 2.36                     | 0.50              |
| 11:A24:403:MET:HA    | 11:A24:406:MET:HE3   | 1.93                     | 0.50              |
| 11:A24:645:GLU:HG2   | 24:D16:867:ASP:OD2   | 2.08                     | 0.50              |
| 10:C24:265:PHE:HE1   | 10:C24:389:LEU:HD12  | 1.76                     | 0.50              |
| 10:C24:931:PRO:HG2   | 10:C24:987:TYR:OH    | 2.10                     | 0.50              |
| 10:C24:962:PHE:HE2   | 10:C24:997:ILE:CD1   | 2.16                     | 0.50              |
| 10:C24:1061:ASN:O    | 10:C24:1063:PRO:HD3  | 2.10                     | 0.50              |
| 10:C24:1553:VAL:HG23 | 10:C24:1592:VAL:HG12 | 1.91                     | 0.50              |
| 11:A40:257:GLN:CD    | 11:A40:263:ASP:CG    | 2.78                     | 0.50              |
| 12:A:400:CYS:SG      | 12:A:423:TYR:HB3     | 2.51                     | 0.50              |
| 12:A:649:LEU:HD21    | 12:A:662:PHE:CE1     | 2.46                     | 0.50              |
| 13:V:825:GLN:CA      | 14:W:707:LYS:HZ1     | 2.23                     | 0.50              |
| 10:C:557:VAL:CG2     | 10:C:565:ARG:NH2     | 2.46                     | 0.50              |
| 10:C:667:ILE:HD12    | 10:C:697:HIS:ND1     | 2.24                     | 0.50              |
| 10:C:1129:VAL:HG12   | 10:C:1130:SER:H      | 1.75                     | 0.50              |
| 10:C8:1061:ASN:O     | 10:C8:1063:PRO:HD3   | 2.10                     | 0.50              |
| 11:A16:257:GLN:CD    | 11:A16:263:ASP:OD1   | 2.51                     | 0.50              |
| 11:A32:150:SER:HB3   | 18:B8:1842:VAL:HG12  | 1.94                     | 0.50              |
| 11:A32:785:HIS:CB    | 11:A32:793:ALA:HB2   | 2.39                     | 0.50              |
| 18:B:789:LEU:CD2     | 18:B:793:LEU:CD1     | 2.85                     | 0.50              |
| 18:B:1745:HIS:C      | 18:B:1747:SER:H      | 2.19                     | 0.50              |
| 18:B8:7:VAL:HG21     | 18:B8:99:ILE:HD11    | 1.91                     | 0.50              |
| 18:B8:330:ALA:HA     | 18:B8:397:PHE:HE2    | 1.75                     | 0.50              |
| 18:B8:671:MET:HE1    | 18:B8:733:VAL:HA     | 1.92                     | 0.50              |
| 19:48:306:ASP:OD1    | 19:48:307:PRO:N      | 2.44                     | 0.50              |
| 21:H:284:LEU:HD21    | 23:J32:650:GLN:HB3   | 1.92                     | 0.50              |
| 21:H:291:VAL:CG2     | 22:I:273:LEU:HD21    | 2.41                     | 0.50              |
| 23:J8:623:GLU:CD     | 23:J8:626:ARG:HH21   | 2.08                     | 0.50              |
| 23:J8:718:GLN:CG     | 23:J8:737:TRP:CH2    | 2.95                     | 0.50              |
| 23:J16:718:GLN:CG    | 23:J16:737:TRP:CH2   | 2.95                     | 0.50              |
| 24:D:275:LYS:HE3     | 24:D:294:GLU:OE1     | 2.11                     | 0.50              |
| 24:D40:843:GLN:NE2   | 24:D40:971:HIS:CE1   | 2.72                     | 0.50              |
| 10:C32:248:LEU:HD11  | 10:C32:260:THR:OG1   | 2.11                     | 0.50              |
| 2:M:278:VAL:HG13     | 2:M:326:GLN:HG3      | 1.91                     | 0.50              |
| 2:M:570:ASP:HA       | 2:M:602:GLN:NE2      | 2.27                     | 0.50              |
| 3:N:29:ALA:HB2       | 3:N:62:VAL:HG13      | 1.94                     | 0.50              |
| 1:R8:982:GLU:OE2     | 24:D40:1436:ARG:O    | 2.30                     | 0.50              |
| 1:R8:1165:MET:CE     | 5:P8:676:GLN:HE21    | 2.24                     | 0.50              |
| 1:R8:1381:GLU:C      | 1:R8:1382:LYS:HG3    | 2.36                     | 0.50              |
| 1:R16:1431:ARG:O     | 2:M16:177:VAL:HG13   | 2.11                     | 0.50              |
| 2:M16:310:HIS:HA     | 2:M16:313:MET:CE     | 2.41                     | 0.50              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M16:570:ASP:HA     | 2:M16:602:GLN:NE2   | 2.27                     | 0.50              |
| 2:M16:625:HIS:HE2    | 3:N16:225:PRO:CB    | 2.23                     | 0.50              |
| 2:M16:810:LEU:CD2    | 2:M16:819:GLN:HG2   | 2.41                     | 0.50              |
| 5:P:233:TYR:CE1      | 5:P:237:MET:HE1     | 2.46                     | 0.50              |
| 5:P:375:LYS:HD3      | 14:W:80:ARG:HH12    | 1.76                     | 0.50              |
| 7:Q:235:ILE:HD13     | 7:Q:243:CYS:HB3     | 1.93                     | 0.50              |
| 5:P8:105:ARG:HD3     | 5:P8:130:VAL:CG2    | 2.42                     | 0.50              |
| 6:O8:119:ARG:CZ      | 6:O8:182:GLU:HA     | 2.38                     | 0.50              |
| 9:K:749:VAL:HG13     | 9:K:752:MET:HE3     | 1.91                     | 0.50              |
| 9:K:1142:ARG:HH21    | 9:K:1204:THR:C      | 2.19                     | 0.50              |
| 9:K8:986:SER:OG      | 9:K8:1012:GLU:HG2   | 2.12                     | 0.50              |
| 10:C16:1624:LEU:HD23 | 10:C16:1628:SER:CB  | 2.37                     | 0.50              |
| 10:C16:1726:PRO:O    | 21:H:275:LYS:CB     | 2.60                     | 0.50              |
| 11:A24:390:ALA:HB1   | 24:D16:1099:ARG:CG  | 2.41                     | 0.50              |
| 11:A24:400:CYS:SG    | 11:A24:423:TYR:HB3  | 2.51                     | 0.50              |
| 10:C24:234:VAL:HG21  | 10:C24:286:ILE:HD13 | 1.93                     | 0.50              |
| 10:C24:386:ASN:O     | 10:C24:390:HIS:HD2  | 1.89                     | 0.50              |
| 13:V:808:LYS:CE      | 15:J:616:ALA:CB     | 2.89                     | 0.50              |
| 14:W:680:ARG:HH22    | 15:J:604:GLU:HG3    | 1.76                     | 0.50              |
| 10:C:1132:SER:OG     | 10:C:1134:TYR:O     | 2.29                     | 0.50              |
| 10:C:1682:VAL:HG22   | 10:C:1758:LEU:HD23  | 1.89                     | 0.50              |
| 10:C8:553:LEU:HD23   | 10:C8:595:THR:HG23  | 1.92                     | 0.50              |
| 10:C8:643:LEU:HB3    | 10:C8:679:ARG:NH1   | 2.27                     | 0.50              |
| 10:C8:1271:PHE:CZ    | 10:C8:1284:ASP:HB3  | 2.37                     | 0.50              |
| 11:A16:150:SER:HB3   | 18:B:1842:VAL:HG12  | 1.93                     | 0.50              |
| 18:B:119:VAL:HG12    | 18:B:119:VAL:O      | 2.11                     | 0.50              |
| 18:B:282:GLU:HG3     | 18:B:444:VAL:HG22   | 1.93                     | 0.50              |
| 18:B:491:VAL:HG12    | 18:B:552:SER:HA     | 1.92                     | 0.50              |
| 18:B:638:ALA:HA      | 18:B:699:MET:CE     | 2.41                     | 0.50              |
| 18:B:684:ILE:HD11    | 24:D16:1065:ALA:HB1 | 1.91                     | 0.50              |
| 18:B:1911:LEU:HB2    | 18:B:1960:LEU:HD13  | 1.92                     | 0.50              |
| 18:B8:1161:LEU:HD21  | 18:B8:1403:ILE:CD1  | 2.37                     | 0.50              |
| 19:4:57:ASN:C        | 19:4:59:GLY:H       | 2.19                     | 0.50              |
| 19:4:59:GLY:C        | 19:4:61:GLU:H       | 2.18                     | 0.50              |
| 20:E8:332:LEU:O      | 20:E8:336:PHE:HD2   | 1.92                     | 0.50              |
| 21:H:288:THR:OG1     | 23:J32:650:GLN:HG2  | 2.11                     | 0.50              |
| 22:I:273:LEU:CD2     | 23:J32:658:LEU:HD21 | 2.41                     | 0.50              |
| 21:H8:193:LEU:HD21   | 21:H8:195:GLN:NE2   | 2.15                     | 0.50              |
| 21:H8:291:VAL:CG2    | 22:I8:273:LEU:HD21  | 2.41                     | 0.50              |
| 22:I8:199:PHE:CG     | 23:J8:620:MET:HG3   | 2.44                     | 0.50              |
| 21:H16:322:LEU:HD22  | 22:I16:300:LEU:HD11 | 1.94                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I16:368:VAL:HG22  | 23:J16:591:LYS:CE    | 2.42                     | 0.50              |
| 10:C32:1033:GLY:CA   | 10:C32:1218:ARG:NH2  | 2.74                     | 0.50              |
| 10:C32:1129:VAL:HG12 | 10:C32:1130:SER:H    | 1.75                     | 0.50              |
| 12:A48:273:ARG:NE    | 12:A48:479:LEU:HD23  | 2.19                     | 0.50              |
| 2:M:773:VAL:CG1      | 2:M:829:ALA:HA       | 2.41                     | 0.50              |
| 2:M:810:LEU:CD2      | 2:M:819:GLN:HG2      | 2.41                     | 0.50              |
| 2:M8:810:LEU:CD2     | 2:M8:819:GLN:HG2     | 2.41                     | 0.50              |
| 2:M16:544:LEU:HD23   | 2:M16:581:LEU:HD22   | 1.94                     | 0.50              |
| 4:T:669:PRO:HG2      | 5:P:702:LEU:CD1      | 2.41                     | 0.50              |
| 5:P:56:ASN:OD1       | 5:P:57:PRO:HD2       | 2.11                     | 0.50              |
| 5:P:217:PHE:CE1      | 5:P:221:LEU:HD11     | 2.46                     | 0.50              |
| 5:P:377:LEU:CD1      | 14:W:23:PRO:HB3      | 2.39                     | 0.50              |
| 6:O:103:MET:CE       | 6:O:124:MET:HE1      | 2.39                     | 0.50              |
| 7:Q:30:ALA:HB1       | 10:C8:815:GLN:NE2    | 2.27                     | 0.50              |
| 7:Q8:114:ASP:O       | 7:Q8:119:ALA:HA      | 2.10                     | 0.50              |
| 7:Q8:327:LEU:HD11    | 7:Q8:358:PHE:HE1     | 1.69                     | 0.50              |
| 6:O16:232:LEU:CD2    | 6:O16:247:VAL:HG22   | 2.41                     | 0.50              |
| 7:Q16:279:LEU:HG     | 7:Q16:313:ILE:HG21   | 1.94                     | 0.50              |
| 8:L16:945:ASN:O      | 9:K16:1282:SER:OG    | 2.30                     | 0.50              |
| 9:K8:1007:GLU:OE1    | 9:K8:1031:LEU:HD21   | 2.11                     | 0.50              |
| 9:K8:1064:PRO:C      | 9:K8:1066:ASP:N      | 2.69                     | 0.50              |
| 10:C24:1023:LEU:CA   | 10:C24:1210:ILE:HD11 | 2.42                     | 0.50              |
| 10:C24:1624:LEU:HD23 | 10:C24:1628:SER:CB   | 2.37                     | 0.50              |
| 10:C24:1733:ARG:NE   | 21:H24:275:LYS:CE    | 2.67                     | 0.50              |
| 13:V:817:GLN:C       | 13:V:819:ALA:H       | 2.18                     | 0.50              |
| 14:W:763:TYR:O       | 14:W:764:SER:C       | 2.49                     | 0.50              |
| 15:J:576:LEU:HD23    | 15:J:576:LEU:O       | 2.12                     | 0.50              |
| 10:C:33:ILE:HG22     | 10:C:158:LEU:HD22    | 1.93                     | 0.50              |
| 10:C:979:MET:HE1     | 10:C:1028:ILE:HB     | 1.94                     | 0.50              |
| 10:C:1211:VAL:HG11   | 10:C:1232:ILE:HG21   | 1.94                     | 0.50              |
| 10:C:1352:GLN:NE2    | 10:C:1357:LEU:CD1    | 2.74                     | 0.50              |
| 10:C8:821:ILE:HD11   | 10:C8:861:ILE:CD1    | 2.42                     | 0.50              |
| 10:C8:1211:VAL:HG11  | 10:C8:1232:ILE:HG21  | 1.93                     | 0.50              |
| 10:C8:1616:ILE:C     | 10:C8:1618:SER:N     | 2.69                     | 0.50              |
| 11:A16:90:PHE:CD2    | 18:B:1788:ILE:CD1    | 2.93                     | 0.50              |
| 11:A16:257:GLN:CD    | 11:A16:263:ASP:CG    | 2.79                     | 0.50              |
| 11:A16:400:CYS:SG    | 11:A16:423:TYR:HB3   | 2.51                     | 0.50              |
| 17:F8:72:SER:C       | 17:F8:74:ILE:N       | 2.69                     | 0.50              |
| 18:B8:1679:ARG:C     | 18:B8:1681:GLN:N     | 2.68                     | 0.50              |
| 23:J24:718:GLN:CG    | 23:J24:737:TRP:CH2   | 2.95                     | 0.50              |
| 22:I16:300:LEU:HD13  | 23:J16:689:LEU:CD2   | 2.40                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:J16:718:GLN:HG3  | 23:J16:737:TRP:CH2  | 2.46                     | 0.50              |
| 24:D40:275:LYS:HE3  | 24:D40:294:GLU:OE1  | 2.11                     | 0.50              |
| 24:D40:275:LYS:CE   | 24:D40:294:GLU:CD   | 2.84                     | 0.50              |
| 10:C32:821:ILE:HD11 | 10:C32:861:ILE:CD1  | 2.42                     | 0.50              |
| 1:R:1431:ARG:O      | 2:M:177:VAL:HG13    | 2.11                     | 0.50              |
| 2:M:310:HIS:HA      | 2:M:313:MET:CE      | 2.41                     | 0.50              |
| 2:M8:335:ALA:O      | 2:M8:336:SER:C      | 2.51                     | 0.50              |
| 2:M8:519:TYR:O      | 2:M8:523:GLY:HA3    | 2.11                     | 0.50              |
| 3:N8:158:TRP:HA     | 3:N8:179:LEU:HD23   | 1.92                     | 0.50              |
| 2:M16:403:LEU:CD2   | 2:M16:425:ALA:HB3   | 2.40                     | 0.50              |
| 2:M16:578:ARG:NH2   | 2:M16:582:GLU:OE2   | 2.44                     | 0.50              |
| 3:N16:177:TYR:HB2   | 3:N16:193:LEU:HB3   | 1.93                     | 0.50              |
| 8:L8:598:LEU:HD21   | 8:L8:627:ARG:HH22   | 1.73                     | 0.50              |
| 8:L8:976:LEU:CD2    | 9:K8:1004:ARG:HD2   | 2.21                     | 0.50              |
| 9:K:648:ALA:O       | 9:K:652:ILE:HG13    | 2.12                     | 0.50              |
| 9:K8:792:LEU:CD1    | 9:K8:849:LEU:HD22   | 2.41                     | 0.50              |
| 10:C16:139:ARG:HG3  | 10:C16:143:LEU:HD12 | 1.92                     | 0.50              |
| 10:C16:1033:GLY:CA  | 10:C16:1218:ARG:NH2 | 2.74                     | 0.50              |
| 11:A24:47:LEU:HD12  | 23:J8:700:LEU:HD11  | 1.93                     | 0.50              |
| 11:A24:326:TYR:CD1  | 17:F:77:TYR:HB3     | 2.13                     | 0.50              |
| 11:A24:587:VAL:HG21 | 11:A24:636:PHE:CE1  | 2.41                     | 0.50              |
| 10:C24:370:ARG:NH2  | 10:C24:446:GLU:OE2  | 2.44                     | 0.50              |
| 10:C24:821:ILE:HD11 | 10:C24:861:ILE:CD1  | 2.42                     | 0.50              |
| 10:C24:1477:GLN:HG2 | 24:D24:1407:PHE:CD1 | 2.47                     | 0.50              |
| 10:C24:1616:ILE:C   | 10:C24:1618:SER:N   | 2.70                     | 0.50              |
| 10:C:26:ARG:HG2     | 10:C:151:LEU:HD13   | 1.93                     | 0.50              |
| 10:C:248:LEU:HD11   | 10:C:260:THR:OG1    | 2.11                     | 0.50              |
| 10:C:286:ILE:HG21   | 10:C:292:PHE:CE1    | 2.45                     | 0.50              |
| 10:C:557:VAL:HA     | 10:C:565:ARG:HE     | 1.75                     | 0.50              |
| 10:C8:370:ARG:NH2   | 10:C8:446:GLU:OE2   | 2.44                     | 0.50              |
| 10:C8:1553:VAL:CG2  | 10:C8:1592:VAL:HG12 | 2.41                     | 0.50              |
| 11:A16:35:ARG:HG2   | 22:I:286:LEU:HD11   | 1.94                     | 0.50              |
| 11:A32:714:GLY:C    | 24:D32:1398:ARG:NH2 | 2.68                     | 0.50              |
| 17:F24:72:SER:C     | 17:F24:74:ILE:N     | 2.69                     | 0.50              |
| 18:B:330:ALA:HA     | 18:B:397:PHE:HE2    | 1.75                     | 0.50              |
| 18:B:609:TYR:CD2    | 18:B:610:VAL:HG23   | 2.45                     | 0.50              |
| 18:B:1161:LEU:HD21  | 18:B:1164:GLU:OE2   | 2.11                     | 0.50              |
| 18:B8:282:GLU:HG3   | 18:B8:444:VAL:HG22  | 1.93                     | 0.50              |
| 18:B8:1575:GLN:NE2  | 24:D32:1403:LEU:CG  | 2.74                     | 0.50              |
| 19:48:185:GLY:C     | 19:48:187:SER:H     | 2.19                     | 0.50              |
| 20:E8:49:THR:HA     | 20:E8:121:VAL:CG1   | 2.40                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:J32:718:GLN:CG    | 23:J32:737:TRP:CH2   | 2.94                     | 0.50              |
| 22:I24:273:LEU:CD2   | 23:J24:658:LEU:HD21  | 2.41                     | 0.50              |
| 21:H16:322:LEU:CG    | 22:I16:300:LEU:HD11  | 2.39                     | 0.50              |
| 24:D32:436:LEU:HD11  | 24:D32:472:ILE:HD12  | 1.94                     | 0.50              |
| 10:C32:265:PHE:HE1   | 10:C32:389:LEU:HD12  | 1.76                     | 0.50              |
| 10:C32:966:CYS:HA    | 10:C32:1025:LEU:HD13 | 1.93                     | 0.50              |
| 10:C32:1624:LEU:CD2  | 10:C32:1632:LEU:HD11 | 2.41                     | 0.50              |
| 10:C32:1637:PHE:CE1  | 12:A48:136:LEU:CD1   | 2.90                     | 0.50              |
| 12:A48:310:GLY:HA3   | 12:A48:313:GLN:OE1   | 2.12                     | 0.50              |
| 12:A48:362:ARG:CD    | 12:A48:366:ARG:CZ    | 2.87                     | 0.50              |
| 2:M:816:ARG:NH2      | 2:M:849:LEU:HB3      | 2.25                     | 0.50              |
| 1:R8:1124:TRP:HZ2    | 4:T8:669:PRO:CD      | 2.24                     | 0.50              |
| 1:R8:1431:ARG:O      | 2:M8:177:VAL:HG13    | 2.11                     | 0.50              |
| 1:R8:1442:THR:HG22   | 3:N8:13:ILE:HD11     | 1.91                     | 0.50              |
| 2:M8:420:CYS:HB3     | 8:L8:391:TRP:CZ3     | 2.46                     | 0.50              |
| 1:R16:1285:PHE:CD2   | 1:R16:1350:LEU:HD22  | 2.46                     | 0.50              |
| 2:M16:519:TYR:O      | 2:M16:523:GLY:HA3    | 2.11                     | 0.50              |
| 2:M16:625:HIS:CD2    | 3:N16:225:PRO:CA     | 2.93                     | 0.50              |
| 5:P:144:THR:C        | 5:P:146:SER:N        | 2.70                     | 0.50              |
| 6:O:54:VAL:HG13      | 6:O:85:TRP:CE2       | 2.45                     | 0.50              |
| 6:O:288:TRP:HZ3      | 6:O:315:TRP:HH2      | 1.59                     | 0.50              |
| 7:Q:327:LEU:HD11     | 7:Q:358:PHE:HE1      | 1.69                     | 0.50              |
| 9:K:975:MET:CE       | 9:K:989:VAL:HG11     | 2.41                     | 0.50              |
| 9:K:986:SER:OG       | 9:K:1012:GLU:HG2     | 2.12                     | 0.50              |
| 9:K:1282:SER:C       | 9:K:1284:MET:H       | 2.20                     | 0.50              |
| 10:C16:370:ARG:NH2   | 10:C16:446:GLU:OE2   | 2.44                     | 0.50              |
| 10:C16:792:PHE:HD1   | 10:C16:850:ARG:CZ    | 2.23                     | 0.50              |
| 10:C16:1708:ARG:HH21 | 10:C16:1733:ARG:NH2  | 2.10                     | 0.50              |
| 10:C16:1757:GLN:HG2  | 11:A24:140:TRP:CD2   | 2.47                     | 0.50              |
| 11:A24:1:MET:C       | 11:A24:3:ASN:H       | 2.20                     | 0.50              |
| 11:A24:20:LEU:HD11   | 21:H8:346:THR:HG23   | 1.91                     | 0.50              |
| 11:A24:803:PRO:CA    | 24:D8:1401:LEU:CD1   | 2.87                     | 0.50              |
| 10:C24:8:VAL:HG23    | 10:C24:133:THR:HG1   | 1.74                     | 0.50              |
| 10:C24:1695:LEU:HD21 | 23:J24:722:LEU:HD21  | 1.94                     | 0.50              |
| 11:A40:798:PHE:HZ    | 11:A40:847:ARG:NH1   | 2.02                     | 0.50              |
| 12:A:634:ILE:HG21    | 12:A:678:LYS:NZ      | 2.26                     | 0.50              |
| 10:C:8:VAL:HG23      | 10:C:133:THR:HG1     | 1.73                     | 0.50              |
| 10:C:300:VAL:CG1     | 10:C:317:ARG:CG      | 2.88                     | 0.50              |
| 10:C8:1033:GLY:CA    | 10:C8:1218:ARG:NH2   | 2.74                     | 0.50              |
| 10:C8:1283:LEU:CD1   | 10:C8:1357:LEU:CD1   | 2.88                     | 0.50              |
| 10:C8:1708:ARG:HH21  | 10:C8:1733:ARG:NH2   | 2.10                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A16:403:MET:HA    | 11:A16:406:MET:HE3   | 1.93                     | 0.50              |
| 11:A32:318:PHE:CE1   | 11:A32:322:ARG:HD2   | 2.47                     | 0.50              |
| 18:B:1575:GLN:CG     | 24:D16:1403:LEU:HD23 | 2.42                     | 0.50              |
| 18:B:1590:LEU:HD22   | 18:B:1620:TRP:HE3    | 1.76                     | 0.50              |
| 18:B:1610:LEU:HA     | 18:B:1613:THR:OG1    | 2.12                     | 0.50              |
| 18:B:1731:PHE:HZ     | 18:B:1749:LEU:HD13   | 1.76                     | 0.50              |
| 18:B:1774:TRP:CE3    | 18:B:1823:ILE:HD13   | 2.46                     | 0.50              |
| 18:B:1856:PHE:CG     | 18:B:1857:PRO:HD2    | 2.47                     | 0.50              |
| 18:B8:609:TYR:CD2    | 18:B8:610:VAL:HG23   | 2.45                     | 0.50              |
| 18:B8:1610:LEU:HA    | 18:B8:1613:THR:OG1   | 2.12                     | 0.50              |
| 18:B8:1856:PHE:CG    | 18:B8:1857:PRO:HD2   | 2.47                     | 0.50              |
| 19:4:51:PRO:O        | 19:4:52:SER:C        | 2.46                     | 0.50              |
| 19:48:163:ALA:HB2    | 19:48:218:LEU:HD11   | 1.92                     | 0.50              |
| 20:E8:432:ILE:HD12   | 24:D40:72:GLU:HG2    | 1.84                     | 0.50              |
| 22:I:289:LEU:CD2     | 22:I:296:ARG:HH12    | 2.17                     | 0.50              |
| 21:H8:322:LEU:HD22   | 22:I8:300:LEU:HD11   | 1.94                     | 0.50              |
| 21:H16:151:LEU:HD12  | 21:H16:194:VAL:HG21  | 1.92                     | 0.50              |
| 24:D:275:LYS:CE      | 24:D:294:GLU:CD      | 2.84                     | 0.50              |
| 10:C32:390:HIS:CE1   | 10:C32:452:LEU:HB3   | 2.44                     | 0.50              |
| 10:C32:1164:VAL:HG13 | 10:C32:1167:PHE:CE2  | 2.46                     | 0.50              |
| 10:C32:1757:GLN:HG2  | 12:A48:140:TRP:CD2   | 2.47                     | 0.50              |
| 1:R:1285:PHE:CD2     | 1:R:1350:LEU:HD22    | 2.46                     | 0.50              |
| 2:M:503:TYR:CD1      | 2:M:507:LEU:HD12     | 2.47                     | 0.50              |
| 2:M:570:ASP:HA       | 2:M:602:GLN:HE22     | 1.76                     | 0.50              |
| 2:M:672:TYR:CB       | 2:M:680:LYS:HZ2      | 2.24                     | 0.50              |
| 2:M8:818:THR:O       | 2:M8:821:THR:OG1     | 2.27                     | 0.50              |
| 3:N8:177:TYR:HB2     | 3:N8:193:LEU:HB3     | 1.93                     | 0.50              |
| 2:M16:166:THR:C      | 2:M16:168:LEU:H      | 2.19                     | 0.50              |
| 2:M16:346:VAL:C      | 2:M16:348:GLU:H      | 2.18                     | 0.50              |
| 2:M16:738:ILE:CD1    | 2:M16:779:SER:CB     | 2.89                     | 0.50              |
| 3:N16:158:TRP:HA     | 3:N16:179:LEU:HD23   | 1.92                     | 0.50              |
| 5:P:96:VAL:HG13      | 5:P:481:ILE:CD1      | 2.35                     | 0.50              |
| 5:P:401:ARG:HD3      | 5:P:414:VAL:CB       | 2.41                     | 0.50              |
| 6:O:105:ASN:ND2      | 6:O:134:ARG:NH2      | 2.59                     | 0.50              |
| 6:O:119:ARG:CZ       | 6:O:182:GLU:HA       | 2.38                     | 0.50              |
| 5:P8:56:ASN:OD1      | 5:P8:57:PRO:HD2      | 2.11                     | 0.50              |
| 7:Q8:331:CYS:HB3     | 7:Q8:352:TRP:CE2     | 2.46                     | 0.50              |
| 7:Q16:235:ILE:HD13   | 7:Q16:243:CYS:HB3    | 1.93                     | 0.50              |
| 8:L:1092:LEU:HD13    | 9:K:999:PHE:HD2      | 1.77                     | 0.50              |
| 9:K8:648:ALA:O       | 9:K8:652:ILE:HG13    | 2.12                     | 0.50              |
| 10:C16:557:VAL:HA    | 10:C16:565:ARG:HE    | 1.75                     | 0.50              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C16:1061:ASN:O    | 10:C16:1063:PRO:HD3 | 2.10                     | 0.50              |
| 10:C16:1624:LEU:HD22 | 10:C16:1628:SER:HB2 | 1.92                     | 0.50              |
| 11:A24:785:HIS:ND1   | 11:A24:793:ALA:HB2  | 2.26                     | 0.50              |
| 10:C24:1033:GLY:CA   | 10:C24:1218:ARG:NH2 | 2.74                     | 0.50              |
| 10:C24:1624:LEU:HD22 | 10:C24:1628:SER:HB2 | 1.92                     | 0.50              |
| 10:C24:1693:LYS:CE   | 10:C24:1749:ASP:OD1 | 2.60                     | 0.50              |
| 11:A40:471:ASN:ND2   | 24:D32:1149:VAL:CB  | 2.73                     | 0.50              |
| 12:A:140:TRP:CD2     | 10:C:1757:GLN:HG2   | 2.47                     | 0.50              |
| 12:A:318:PHE:CE1     | 12:A:322:ARG:HD2    | 2.47                     | 0.50              |
| 13:V:808:LYS:NZ      | 15:J:616:ALA:CB     | 2.74                     | 0.50              |
| 10:C:265:PHE:HE1     | 10:C:389:LEU:HD12   | 1.76                     | 0.50              |
| 10:C:821:ILE:HD11    | 10:C:861:ILE:CD1    | 2.42                     | 0.50              |
| 10:C:861:ILE:HG22    | 10:C:861:ILE:O      | 2.11                     | 0.50              |
| 10:C:1164:VAL:HG13   | 10:C:1167:PHE:CE2   | 2.46                     | 0.50              |
| 10:C8:37:PHE:N       | 10:C8:38:PRO:CD     | 2.74                     | 0.50              |
| 10:C8:453:LEU:HB3    | 10:C8:486:LEU:HD21  | 1.90                     | 0.50              |
| 10:C8:520:TYR:OH     | 10:C8:542:ASP:OD2   | 2.23                     | 0.50              |
| 10:C8:561:ASN:OD1    | 10:C8:562:PRO:CD    | 2.50                     | 0.50              |
| 10:C8:1132:SER:OG    | 10:C8:1134:TYR:O    | 2.29                     | 0.50              |
| 10:C8:1591:LYS:NZ    | 16:A8:139:ASP:OD2   | 2.34                     | 0.50              |
| 10:C8:1703:ILE:CD1   | 10:C8:1741:MET:HE2  | 2.42                     | 0.50              |
| 10:C8:1757:GLN:HG2   | 16:A8:140:TRP:CD2   | 2.47                     | 0.50              |
| 11:A16:318:PHE:CE1   | 11:A16:322:ARG:HD2  | 2.47                     | 0.50              |
| 18:B:313:ILE:HD13    | 18:B:331:TRP:HB2    | 1.92                     | 0.50              |
| 18:B:345:GLU:HA      | 18:B:351:MET:CE     | 2.35                     | 0.50              |
| 18:B:463:SER:O       | 18:B:467:ILE:HG12   | 2.11                     | 0.50              |
| 18:B:1139:LYS:CB     | 18:B:1365:ARG:HH11  | 2.23                     | 0.50              |
| 18:B8:1265:PHE:O     | 18:B8:1269:THR:HG23 | 2.12                     | 0.50              |
| 19:4:103:GLN:OE1     | 19:4:411:LEU:HD13   | 2.09                     | 0.50              |
| 21:H16:239:SER:HB3   | 23:J16:603:LEU:HD21 | 1.93                     | 0.50              |
| 21:H16:255:LEU:HD13  | 23:J16:655:GLU:OE2  | 2.01                     | 0.50              |
| 21:H16:288:THR:OG1   | 23:J16:650:GLN:HG2  | 2.11                     | 0.50              |
| 24:D:405:GLN:NE2     | 24:D16:752:VAL:CG2  | 2.74                     | 0.50              |
| 24:D8:274:MET:CE     | 24:D8:321:SER:HB2   | 2.40                     | 0.50              |
| 24:D8:552:VAL:HG21   | 24:D8:592:ILE:CD1   | 2.42                     | 0.50              |
| 24:D16:275:LYS:CE    | 24:D16:294:GLU:CD   | 2.84                     | 0.50              |
| 24:D24:436:LEU:HD11  | 24:D24:472:ILE:HD12 | 1.94                     | 0.50              |
| 24:D32:275:LYS:CE    | 24:D32:294:GLU:CD   | 2.84                     | 0.50              |
| 24:D32:1452:LYS:HE2  | 24:D32:1456:GLU:OE1 | 2.11                     | 0.50              |
| 10:C32:37:PHE:N      | 10:C32:38:PRO:CD    | 2.73                     | 0.50              |
| 10:C32:370:ARG:NH2   | 10:C32:446:GLU:OE2  | 2.44                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1211:VAL:HG11 | 10:C32:1232:ILE:HG21 | 1.94                     | 0.50              |
| 1:R:1191:LYS:CB      | 24:D:1453:GLU:CD     | 2.85                     | 0.50              |
| 1:R:1266:THR:CA      | 5:P:684:ARG:NH2      | 2.74                     | 0.50              |
| 1:R:1421:ALA:HB1     | 6:O:162:THR:HG22     | 1.92                     | 0.50              |
| 1:R:1425:PRO:C       | 6:O:165:LYS:HZ1      | 2.19                     | 0.50              |
| 2:M:166:THR:N        | 2:M:169:THR:HG1      | 2.08                     | 0.50              |
| 1:R8:768:LEU:CD1     | 24:D40:1362:VAL:O    | 2.58                     | 0.50              |
| 2:M8:738:ILE:CD1     | 2:M8:779:SER:CB      | 2.89                     | 0.50              |
| 1:R16:1112:LYS:NZ    | 1:R16:1156:GLU:OE1   | 2.29                     | 0.50              |
| 1:R16:1381:GLU:C     | 1:R16:1382:LYS:HG3   | 2.36                     | 0.50              |
| 1:R16:1463:GLN:CA    | 6:O16:160:LEU:HD21   | 2.35                     | 0.50              |
| 2:M16:335:ALA:O      | 2:M16:336:SER:C      | 2.51                     | 0.50              |
| 5:P:112:LEU:HD13     | 14:W:17:SER:HA       | 1.93                     | 0.50              |
| 6:O:42:SER:HB2       | 7:Q:40:TYR:OH        | 2.12                     | 0.50              |
| 7:Q:279:LEU:HG       | 7:Q:313:ILE:HG21     | 1.94                     | 0.50              |
| 5:P16:479:ALA:N      | 5:P16:480:PRO:CD     | 2.75                     | 0.50              |
| 9:K:1085:TYR:HE1     | 9:K:1093:SER:O       | 1.86                     | 0.50              |
| 9:K:1279:GLU:O       | 9:K:1280:PHE:C       | 2.50                     | 0.50              |
| 9:K8:955:TYR:OH      | 9:K8:984:GLY:CA      | 2.60                     | 0.50              |
| 10:C16:1132:SER:OG   | 10:C16:1134:TYR:O    | 2.29                     | 0.50              |
| 10:C16:1352:GLN:NE2  | 10:C16:1357:LEU:CD1  | 2.74                     | 0.50              |
| 11:A24:51:THR:CG2    | 22:I8:317:HIS:HB2    | 2.42                     | 0.50              |
| 11:A24:362:ARG:CD    | 11:A24:366:ARG:CZ    | 2.87                     | 0.50              |
| 10:C24:1352:GLN:NE2  | 10:C24:1357:LEU:CD1  | 2.74                     | 0.50              |
| 11:A40:560:MET:HE2   | 11:A40:615:GLN:NE2   | 1.97                     | 0.50              |
| 12:A:643:SER:HA      | 12:A:682:LEU:HD23    | 1.94                     | 0.50              |
| 13:V:798:LEU:HD12    | 15:J:606:ILE:CG1     | 2.42                     | 0.50              |
| 10:C:1293:THR:CG2    | 10:C:1369:LEU:HD13   | 2.42                     | 0.50              |
| 10:C8:248:LEU:HD11   | 10:C8:260:THR:OG1    | 2.11                     | 0.50              |
| 10:C8:643:LEU:CD1    | 10:C8:656:THR:OG1    | 2.60                     | 0.50              |
| 10:C8:1023:LEU:CA    | 10:C8:1210:ILE:HD11  | 2.42                     | 0.50              |
| 11:A16:54:ASN:O      | 11:A16:59:GLN:CD     | 2.54                     | 0.50              |
| 18:B:907:SER:C       | 18:B:909:LEU:N       | 2.69                     | 0.50              |
| 18:B:1911:LEU:HB2    | 18:B:1960:LEU:HD12   | 1.91                     | 0.50              |
| 18:B8:7:VAL:HG11     | 18:B8:99:ILE:CD1     | 2.41                     | 0.50              |
| 18:B8:771:MET:HE3    | 18:B8:840:VAL:CG2    | 2.41                     | 0.50              |
| 18:B8:1142:PHE:CE2   | 18:B8:1348:VAL:CG1   | 2.93                     | 0.50              |
| 18:B8:1679:ARG:O     | 18:B8:1681:GLN:N     | 2.41                     | 0.50              |
| 19:48:59:GLY:C       | 19:48:61:GLU:H       | 2.18                     | 0.50              |
| 19:48:329:SER:OG     | 19:48:333:SER:HB3    | 2.12                     | 0.50              |
| 21:H8:239:SER:HB3    | 23:J8:603:LEU:HD21   | 1.93                     | 0.50              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D8:275:LYS:HE3    | 24:D8:294:GLU:OE1    | 2.11                     | 0.50              |
| 24:D16:436:LEU:HD11  | 24:D16:472:ILE:HD12  | 1.94                     | 0.50              |
| 10:C32:1167:PHE:C    | 10:C32:1169:ASN:N    | 2.70                     | 0.50              |
| 10:C32:1258:LEU:CA   | 10:C32:1323:LEU:CD1  | 2.90                     | 0.50              |
| 1:R8:1265:PHE:CD2    | 1:R8:1269:LEU:HD12   | 2.45                     | 0.50              |
| 2:M8:486:MET:HG3     | 2:M8:499:ILE:HD13    | 1.94                     | 0.50              |
| 2:M8:503:TYR:CD1     | 2:M8:507:LEU:HD12    | 2.47                     | 0.50              |
| 2:M8:570:ASP:HA      | 2:M8:602:GLN:HE22    | 1.76                     | 0.50              |
| 2:M8:820:LEU:HG      | 4:T8:656:TRP:CZ2     | 2.47                     | 0.50              |
| 3:N16:9:GLY:C        | 3:N16:36:LYS:HZ1     | 2.20                     | 0.50              |
| 5:P:175:MET:CE       | 5:P:436:ALA:HB2      | 2.38                     | 0.50              |
| 5:P:193:VAL:HG21     | 5:P:368:LEU:HD21     | 1.93                     | 0.50              |
| 5:P8:217:PHE:CE1     | 5:P8:221:LEU:HD11    | 2.46                     | 0.50              |
| 5:P8:247:GLU:N       | 5:P8:247:GLU:CD      | 2.70                     | 0.50              |
| 6:O8:42:SER:HB2      | 7:Q8:40:TYR:OH       | 2.12                     | 0.50              |
| 6:O8:232:LEU:CD2     | 6:O8:247:VAL:HG22    | 2.41                     | 0.50              |
| 8:L16:1069:LEU:CD2   | 9:K16:1086:VAL:HG21  | 2.41                     | 0.50              |
| 9:K8:716:ALA:C       | 10:C32:503:THR:HG21  | 2.37                     | 0.50              |
| 9:K16:792:LEU:CG     | 9:K16:864:ILE:HD11   | 2.42                     | 0.50              |
| 10:C16:470:HIS:CD2   | 10:C16:508:ILE:HD11  | 2.44                     | 0.50              |
| 10:C16:1293:THR:CG2  | 10:C16:1369:LEU:HD13 | 2.42                     | 0.50              |
| 11:A24:72:ILE:HD11   | 21:H8:348:ALA:HA     | 1.94                     | 0.50              |
| 10:C24:22:THR:HB     | 10:C24:23:PRO:HD2    | 1.92                     | 0.50              |
| 10:C24:26:ARG:CZ     | 10:C24:148:GLU:OE2   | 2.60                     | 0.50              |
| 10:C24:1211:VAL:HG11 | 10:C24:1232:ILE:HG21 | 1.94                     | 0.50              |
| 11:A40:310:GLY:HA3   | 11:A40:313:GLN:OE1   | 2.12                     | 0.50              |
| 11:A40:381:TRP:CD1   | 11:A40:386:GLY:HA2   | 2.46                     | 0.50              |
| 11:A40:403:MET:HA    | 11:A40:406:MET:HE3   | 1.93                     | 0.50              |
| 10:C:370:ARG:NH2     | 10:C:446:GLU:OE2     | 2.44                     | 0.50              |
| 10:C:1010:ALA:N      | 10:C:1192:ARG:HH21   | 1.81                     | 0.50              |
| 10:C:1553:VAL:CG2    | 10:C:1592:VAL:HG12   | 2.41                     | 0.50              |
| 10:C8:1693:LYS:CE    | 10:C8:1749:ASP:OD1   | 2.60                     | 0.50              |
| 11:A32:28:SER:C      | 11:A32:30:PHE:N      | 2.70                     | 0.50              |
| 11:A32:381:TRP:CD1   | 11:A32:386:GLY:HA2   | 2.46                     | 0.50              |
| 11:A32:403:MET:HA    | 11:A32:406:MET:HE3   | 1.93                     | 0.50              |
| 18:B:690:TRP:CH2     | 18:B:787:VAL:CG2     | 2.94                     | 0.50              |
| 18:B:1265:PHE:O      | 18:B:1269:THR:HG23   | 2.12                     | 0.50              |
| 18:B:1783:VAL:O      | 18:B:1783:VAL:HG12   | 2.11                     | 0.50              |
| 18:B8:814:GLU:O      | 18:B8:818:SER:OG     | 2.30                     | 0.50              |
| 18:B8:1175:ALA:CB    | 18:B8:1325:MET:HE2   | 2.42                     | 0.50              |
| 18:B8:1736:ALA:HA    | 18:B8:1777:LEU:CD1   | 2.42                     | 0.50              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B8:1753:PRO:HG3   | 18:B8:1762:CYS:SG   | 2.52                     | 0.50              |
| 19:4:306:ASP:OD1     | 19:4:307:PRO:N      | 2.44                     | 0.50              |
| 21:H16:366:MET:HE3   | 22:I16:332:MET:CE   | 2.32                     | 0.50              |
| 24:D32:552:VAL:HG21  | 24:D32:592:ILE:CD1  | 2.42                     | 0.50              |
| 10:C32:26:ARG:CZ     | 10:C32:148:GLU:OE2  | 2.60                     | 0.50              |
| 10:C32:1017:HIS:NE2  | 10:C32:1139:ARG:HD3 | 2.27                     | 0.50              |
| 12:A48:381:TRP:CD1   | 12:A48:386:GLY:HA2  | 2.46                     | 0.50              |
| 1:R:1124:TRP:HZ2     | 4:T:669:PRO:CD      | 2.24                     | 0.49              |
| 3:N:116:ILE:HG23     | 3:N:177:TYR:CZ      | 2.47                     | 0.49              |
| 3:N8:19:MET:CE       | 3:N8:23:GLY:HA2     | 2.40                     | 0.49              |
| 3:N8:29:ALA:HB2      | 3:N8:62:VAL:HG13    | 1.94                     | 0.49              |
| 2:M16:570:ASP:HA     | 2:M16:602:GLN:HE22  | 1.76                     | 0.49              |
| 2:M16:818:THR:O      | 2:M16:821:THR:OG1   | 2.27                     | 0.49              |
| 6:O:232:LEU:CD2      | 6:O:247:VAL:HG22    | 2.41                     | 0.49              |
| 5:P8:233:TYR:CE1     | 5:P8:237:MET:HE1    | 2.47                     | 0.49              |
| 7:Q8:33:ARG:HH22     | 7:Q8:345:ASP:HB3    | 1.77                     | 0.49              |
| 7:Q16:52:GLN:OE1     | 7:Q16:68:ILE:HG21   | 2.11                     | 0.49              |
| 7:Q16:88:ASN:O       | 7:Q16:89:GLY:O      | 2.29                     | 0.49              |
| 7:Q16:331:CYS:HB3    | 7:Q16:352:TRP:CE2   | 2.46                     | 0.49              |
| 9:K:1019:ARG:CZ      | 9:K:1059:ARG:CD     | 2.89                     | 0.49              |
| 9:K8:994:TYR:CE2     | 9:K8:1023:LEU:CD1   | 2.95                     | 0.49              |
| 9:K8:1048:GLN:CD     | 9:K8:1128:ARG:CG    | 2.79                     | 0.49              |
| 9:K8:1282:SER:C      | 9:K8:1284:MET:H     | 2.20                     | 0.49              |
| 9:K16:975:MET:HG3    | 9:K16:985:PHE:CE1   | 2.47                     | 0.49              |
| 10:C16:821:ILE:HD11  | 10:C16:861:ILE:CD1  | 2.42                     | 0.49              |
| 10:C16:1285:VAL:HG21 | 10:C16:1738:MET:HE2 | 0.51                     | 0.49              |
| 11:A24:35:ARG:HG2    | 22:I8:286:LEU:HD11  | 1.94                     | 0.49              |
| 11:A24:318:PHE:CE1   | 11:A24:322:ARG:HD2  | 2.47                     | 0.49              |
| 11:A24:643:SER:O     | 11:A24:659:ARG:HD2  | 2.12                     | 0.49              |
| 10:C24:1132:SER:OG   | 10:C24:1134:TYR:O   | 2.29                     | 0.49              |
| 10:C24:1166:SER:C    | 10:C24:1168:PRO:N   | 2.70                     | 0.49              |
| 10:C24:1708:ARG:HH22 | 21:H24:275:LYS:HG2  | 0.46                     | 0.49              |
| 10:C24:1757:GLN:HG2  | 11:A40:140:TRP:CD2  | 2.47                     | 0.49              |
| 11:A40:47:LEU:HD12   | 23:J16:700:LEU:HD11 | 1.93                     | 0.49              |
| 11:A40:48:LYS:HE3    | 22:I16:313:ASP:OD2  | 2.12                     | 0.49              |
| 11:A40:318:PHE:CE1   | 11:A40:322:ARG:HD2  | 2.47                     | 0.49              |
| 12:A:587:VAL:HG22    | 12:A:627:ILE:HD13   | 1.95                     | 0.49              |
| 10:C:1258:LEU:CA     | 10:C:1323:LEU:CD1   | 2.90                     | 0.49              |
| 10:C:1283:LEU:CD1    | 10:C:1357:LEU:HD11  | 2.40                     | 0.49              |
| 10:C:1624:LEU:CD2    | 10:C:1632:LEU:HD11  | 2.41                     | 0.49              |
| 10:C8:300:VAL:CG1    | 10:C8:317:ARG:CG    | 2.88                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:90:ILE:HD11    | 18:B:131:ILE:CD1    | 2.42                     | 0.49              |
| 18:B:109:MET:HE1    | 18:B:120:ALA:HB2    | 1.94                     | 0.49              |
| 18:B:1174:ALA:HA    | 18:B:1249:LEU:HD11  | 1.94                     | 0.49              |
| 18:B:1684:TRP:CH2   | 18:B:1752:PRO:CG    | 2.95                     | 0.49              |
| 18:B:1736:ALA:HA    | 18:B:1777:LEU:CD1   | 2.42                     | 0.49              |
| 18:B8:503:SER:H     | 18:B8:504:PRO:CD    | 2.24                     | 0.49              |
| 18:B8:1543:HIS:O    | 18:B8:1547:GLN:HG2  | 2.12                     | 0.49              |
| 18:B8:1731:PHE:HZ   | 18:B8:1749:LEU:HD13 | 1.76                     | 0.49              |
| 18:B8:1783:VAL:O    | 18:B8:1783:VAL:HG12 | 2.11                     | 0.49              |
| 19:48:305:TRP:CE2   | 19:48:312:ILE:HD12  | 2.46                     | 0.49              |
| 21:H24:239:SER:HB3  | 23:J24:603:LEU:HD21 | 1.93                     | 0.49              |
| 22:I24:300:LEU:HD11 | 23:J24:689:LEU:HD21 | 1.91                     | 0.49              |
| 22:I24:328:TYR:CE1  | 23:J24:717:ILE:CG2  | 2.95                     | 0.49              |
| 24:D8:1452:LYS:HE2  | 24:D8:1456:GLU:OE1  | 2.11                     | 0.49              |
| 24:D24:275:LYS:CE   | 24:D24:294:GLU:CD   | 2.84                     | 0.49              |
| 24:D24:857:THR:OG1  | 24:D24:889:LEU:HD13 | 2.11                     | 0.49              |
| 24:D40:552:VAL:HG21 | 24:D40:592:ILE:CD1  | 2.42                     | 0.49              |
| 10:C32:855:VAL:HB   | 10:C32:856:PRO:HD3  | 1.94                     | 0.49              |
| 10:C32:1111:SER:OG  | 10:C32:1114:TYR:HD2 | 1.95                     | 0.49              |
| 12:A48:318:PHE:CE1  | 12:A48:322:ARG:HD2  | 2.47                     | 0.49              |
| 1:R:1075:LYS:HZ3    | 1:R:1079:ASP:CG     | 2.19                     | 0.49              |
| 1:R:1459:ARG:HG2    | 10:C:731:GLN:NE2    | 2.27                     | 0.49              |
| 2:M:166:THR:C       | 2:M:168:LEU:H       | 2.19                     | 0.49              |
| 2:M:447:LEU:HD21    | 8:L:280:GLN:HE22    | 1.76                     | 0.49              |
| 1:R8:1033:LYS:HE3   | 1:R8:1037:ASP:OD2   | 2.12                     | 0.49              |
| 1:R8:1285:PHE:CD2   | 1:R8:1350:LEU:HD22  | 2.46                     | 0.49              |
| 2:M8:339:GLU:O      | 2:M8:341:ASP:N      | 2.44                     | 0.49              |
| 1:R16:1182:PRO:C    | 1:R16:1184:GLU:N    | 2.68                     | 0.49              |
| 2:M16:567:ASP:OD1   | 2:M16:568:PRO:HD2   | 2.12                     | 0.49              |
| 4:T8:671:ILE:CD1    | 5:P8:698:GLY:HA3    | 2.42                     | 0.49              |
| 5:P:607:PHE:CE2     | 5:P:611:LEU:CD1     | 2.96                     | 0.49              |
| 7:Q:52:GLN:OE1      | 7:Q:68:ILE:HG21     | 2.11                     | 0.49              |
| 7:Q:341:GLN:CD      | 10:C8:751:ARG:HH12  | 2.13                     | 0.49              |
| 5:P8:5:SER:O        | 5:P8:7:GLU:N        | 2.44                     | 0.49              |
| 6:O8:23:ARG:CZ      | 6:O8:37:GLU:OE1     | 2.61                     | 0.49              |
| 5:P16:5:SER:O       | 5:P16:7:GLU:N       | 2.44                     | 0.49              |
| 5:P16:96:VAL:HG13   | 5:P16:481:ILE:CD1   | 2.35                     | 0.49              |
| 5:P16:154:ASP:OD1   | 5:P16:155:PRO:HD2   | 2.11                     | 0.49              |
| 5:P16:233:TYR:CE1   | 5:P16:237:MET:HE1   | 2.47                     | 0.49              |
| 5:P16:543:GLY:HA2   | 5:P16:587:LEU:HD13  | 1.95                     | 0.49              |
| 7:Q16:78:SER:OG     | 7:Q16:103:THR:HB    | 2.12                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 8:L:1092:LEU:HD13    | 9:K:999:PHE:CD2      | 2.47                     | 0.49              |
| 9:K8:1230:LEU:CD2    | 9:K8:1244:VAL:HG22   | 2.34                     | 0.49              |
| 10:C16:26:ARG:CZ     | 10:C16:148:GLU:OE2   | 2.60                     | 0.49              |
| 10:C16:717:GLU:HG3   | 23:J8:656:ARG:NE     | 2.26                     | 0.49              |
| 10:C16:861:ILE:HG22  | 10:C16:861:ILE:O     | 2.11                     | 0.49              |
| 10:C16:1017:HIS:NE2  | 10:C16:1139:ARG:HD3  | 2.27                     | 0.49              |
| 10:C16:1074:LEU:CD1  | 10:C16:1074:LEU:C    | 2.77                     | 0.49              |
| 10:C16:1166:SER:C    | 10:C16:1168:PRO:N    | 2.70                     | 0.49              |
| 10:C24:139:ARG:HG3   | 10:C24:143:LEU:HD12  | 1.92                     | 0.49              |
| 10:C24:1129:VAL:HG12 | 10:C24:1130:SER:H    | 1.76                     | 0.49              |
| 13:V:730:GLN:HB2     | 13:V:731:PRO:HD3     | 1.94                     | 0.49              |
| 14:W:694:CYS:HB3     | 15:J:617:LEU:HD22    | 1.95                     | 0.49              |
| 10:C:35:ASN:CB       | 24:D:1148:LEU:HD11   | 2.42                     | 0.49              |
| 10:C:277:SER:O       | 10:C:280:SER:N       | 2.35                     | 0.49              |
| 10:C:1017:HIS:NE2    | 10:C:1139:ARG:HD3    | 2.27                     | 0.49              |
| 10:C8:1250:ALA:CB    | 10:C8:1309:ARG:HH11  | 2.23                     | 0.49              |
| 10:C8:1285:VAL:HG21  | 10:C8:1738:MET:HE2   | 0.50                     | 0.49              |
| 11:A16:381:TRP:CD1   | 11:A16:386:GLY:HA2   | 2.46                     | 0.49              |
| 11:A32:35:ARG:HG2    | 22:I24:286:LEU:HD11  | 1.94                     | 0.49              |
| 11:A32:47:LEU:HD12   | 23:J24:700:LEU:HD11  | 1.93                     | 0.49              |
| 11:A32:54:ASN:O      | 11:A32:59:GLN:CD     | 2.54                     | 0.49              |
| 18:B:7:VAL:HG12      | 18:B:8:ASP:H         | 1.76                     | 0.49              |
| 18:B:424:SER:O       | 18:B:428:GLN:HB2     | 2.12                     | 0.49              |
| 18:B:1685:THR:HG22   | 18:B:1689:TYR:CD1    | 2.46                     | 0.49              |
| 18:B8:254:LEU:O      | 18:B8:256:VAL:HG23   | 2.13                     | 0.49              |
| 18:B8:907:SER:C      | 18:B8:909:LEU:N      | 2.69                     | 0.49              |
| 19:4:232:TYR:CD2     | 19:4:233:ASP:OD1     | 2.65                     | 0.49              |
| 20:E:494:ILE:HD13    | 20:E:507:LEU:HB3     | 1.94                     | 0.49              |
| 19:48:294:SER:C      | 19:48:296:GLY:H      | 2.20                     | 0.49              |
| 20:E8:438:SER:O      | 20:E8:440:VAL:N      | 2.43                     | 0.49              |
| 21:H24:322:LEU:HD22  | 22:I24:300:LEU:HD11  | 1.94                     | 0.49              |
| 22:I24:199:PHE:CG    | 23:J24:620:MET:HG3   | 2.44                     | 0.49              |
| 22:I16:199:PHE:CG    | 23:J16:620:MET:HG3   | 2.43                     | 0.49              |
| 24:D8:436:LEU:HD11   | 24:D8:472:ILE:HD12   | 1.94                     | 0.49              |
| 10:C32:26:ARG:NH2    | 10:C32:151:LEU:HB2   | 2.24                     | 0.49              |
| 10:C32:286:ILE:HG21  | 10:C32:292:PHE:CE1   | 2.45                     | 0.49              |
| 10:C32:420:TYR:CZ    | 10:C32:435:SER:HB3   | 2.47                     | 0.49              |
| 10:C32:699:HIS:O     | 10:C32:703:SER:OG    | 2.23                     | 0.49              |
| 10:C32:1023:LEU:CA   | 10:C32:1210:ILE:HD11 | 2.42                     | 0.49              |
| 12:A48:440:LEU:CG    | 12:A48:443:LEU:HD11  | 2.39                     | 0.49              |
| 2:M:173:SER:HG       | 3:N:234:GLN:HE22     | 1.58                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M:185:ARG:HH11     | 2:M:213:LEU:HD13     | 1.68                     | 0.49              |
| 2:M:328:THR:HG21     | 2:M:350:SER:HB2      | 1.94                     | 0.49              |
| 2:M:344:GLN:O        | 2:M:345:ASP:C        | 2.44                     | 0.49              |
| 2:M8:185:ARG:HH11    | 2:M8:213:LEU:HD13    | 1.68                     | 0.49              |
| 2:M8:567:ASP:OD1     | 2:M8:568:PRO:HD2     | 2.12                     | 0.49              |
| 2:M8:625:HIS:CD2     | 3:N8:225:PRO:CA      | 2.93                     | 0.49              |
| 2:M16:328:THR:HG21   | 2:M16:350:SER:HB2    | 1.94                     | 0.49              |
| 2:M16:651:ARG:HG3    | 2:M16:664:MET:CE     | 2.42                     | 0.49              |
| 5:P:167:SER:HB3      | 5:P:398:LYS:HE3      | 1.94                     | 0.49              |
| 5:P8:144:THR:C       | 5:P8:146:SER:N       | 2.70                     | 0.49              |
| 7:Q8:78:SER:OG       | 7:Q8:103:THR:HB      | 2.11                     | 0.49              |
| 8:L:1074:ARG:CD      | 9:K:1089:LYS:HB2     | 2.43                     | 0.49              |
| 8:L16:1074:ARG:NH1   | 9:K16:1089:LYS:HD2   | 2.21                     | 0.49              |
| 9:K:719:GLY:CA       | 9:K:720:SER:N        | 2.70                     | 0.49              |
| 9:K:994:TYR:CE2      | 9:K:1023:LEU:CD1     | 2.95                     | 0.49              |
| 10:C16:1002:LEU:HD23 | 10:C16:1012:ARG:NH1  | 2.26                     | 0.49              |
| 10:C16:1023:LEU:CA   | 10:C16:1210:ILE:HD11 | 2.42                     | 0.49              |
| 10:C16:1258:LEU:CA   | 10:C16:1323:LEU:CD1  | 2.90                     | 0.49              |
| 11:A24:310:GLY:HA3   | 11:A24:313:GLN:OE1   | 2.12                     | 0.49              |
| 10:C24:1111:SER:OG   | 10:C24:1114:TYR:HD2  | 1.95                     | 0.49              |
| 10:C24:1708:ARG:HH21 | 10:C24:1733:ARG:NH2  | 2.10                     | 0.49              |
| 11:A40:35:ARG:HG2    | 22:I16:286:LEU:HD11  | 1.94                     | 0.49              |
| 11:A40:749:GLN:HE21  | 24:D24:1398:ARG:CD   | 2.24                     | 0.49              |
| 10:C:153:ALA:O       | 24:D:1403:LEU:HD11   | 2.12                     | 0.49              |
| 10:C:717:GLU:O       | 10:C:718:HIS:C       | 2.41                     | 0.49              |
| 10:C8:855:VAL:HB     | 10:C8:856:PRO:HD3    | 1.94                     | 0.49              |
| 10:C8:959:GLU:CG     | 10:C8:1139:ARG:HE    | 2.24                     | 0.49              |
| 10:C8:1167:PHE:C     | 10:C8:1169:ASN:N     | 2.70                     | 0.49              |
| 10:C8:1283:LEU:HD11  | 10:C8:1357:LEU:HD13  | 1.91                     | 0.49              |
| 11:A16:54:ASN:CB     | 11:A16:59:GLN:HE22   | 2.21                     | 0.49              |
| 11:A16:124:ASN:HA    | 18:B:1523:ARG:HH11   | 1.78                     | 0.49              |
| 11:A16:587:VAL:HG22  | 11:A16:627:ILE:HD13  | 1.94                     | 0.49              |
| 18:B:1424:LEU:CD2    | 18:B:1490:ILE:CD1    | 2.90                     | 0.49              |
| 18:B8:1174:ALA:HA    | 18:B8:1249:LEU:HD11  | 1.94                     | 0.49              |
| 18:B8:1424:LEU:CD2   | 18:B8:1490:ILE:CD1   | 2.90                     | 0.49              |
| 19:48:362:ALA:HB3    | 19:48:417:ASP:OD2    | 2.12                     | 0.49              |
| 21:H:284:LEU:HD21    | 23:J32:647:MET:O     | 2.13                     | 0.49              |
| 21:H:322:LEU:HD22    | 22:I:300:LEU:HD11    | 1.94                     | 0.49              |
| 21:H8:154:VAL:HG11   | 21:H8:188:ARG:HE     | 1.77                     | 0.49              |
| 22:I8:178:LEU:HD12   | 23:J8:599:LEU:HD22   | 1.95                     | 0.49              |
| 22:I24:300:LEU:CG    | 23:J24:689:LEU:HD21  | 2.41                     | 0.49              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 22:I16:368:VAL:HG21 | 23:J16:591:LYS:NZ    | 2.27                     | 0.49              |
| 24:D:552:VAL:HG21   | 24:D:592:ILE:CD1     | 2.42                     | 0.49              |
| 24:D40:839:GLU:HG2  | 24:D40:971:HIS:CD2   | 2.46                     | 0.49              |
| 10:C32:390:HIS:CB   | 10:C32:452:LEU:CB    | 2.85                     | 0.49              |
| 10:C32:1271:PHE:CD1 | 10:C32:1731:HIS:NE2  | 2.75                     | 0.49              |
| 10:C32:1693:LYS:CE  | 10:C32:1749:ASP:OD1  | 2.60                     | 0.49              |
| 10:C32:1703:ILE:CD1 | 10:C32:1741:MET:HE2  | 2.42                     | 0.49              |
| 10:C32:1805:ASP:OD1 | 10:C32:1830:LYS:NZ   | 2.27                     | 0.49              |
| 2:M8:570:ASP:HA     | 2:M8:602:GLN:NE2     | 2.27                     | 0.49              |
| 2:M8:632:VAL:CG2    | 3:N8:222:LEU:O       | 2.61                     | 0.49              |
| 2:M16:544:LEU:HD11  | 2:M16:586:ALA:CA     | 2.43                     | 0.49              |
| 2:M16:632:VAL:CG2   | 3:N16:222:LEU:O      | 2.61                     | 0.49              |
| 3:N16:167:LEU:HD23  | 3:N16:169:SER:HB2    | 1.95                     | 0.49              |
| 5:P:543:GLY:HA2     | 5:P:587:LEU:HD13     | 1.95                     | 0.49              |
| 5:P8:193:VAL:HG21   | 5:P8:368:LEU:HD21    | 1.93                     | 0.49              |
| 5:P8:592:SER:C      | 5:P8:594:ILE:N       | 2.56                     | 0.49              |
| 5:P8:607:PHE:CE2    | 5:P8:611:LEU:CD1     | 2.96                     | 0.49              |
| 6:O8:303:MET:HE1    | 6:O8:322:GLU:HG3     | 1.95                     | 0.49              |
| 7:Q8:235:ILE:HD13   | 7:Q8:243:CYS:HB3     | 1.93                     | 0.49              |
| 5:P16:56:ASN:OD1    | 5:P16:57:PRO:HD2     | 2.11                     | 0.49              |
| 5:P16:144:THR:C     | 5:P16:146:SER:N      | 2.70                     | 0.49              |
| 6:O16:103:MET:CE    | 6:O16:124:MET:HE1    | 2.39                     | 0.49              |
| 8:L8:1064:ASP:OD1   | 9:K8:1101:GLU:OE1    | 2.29                     | 0.49              |
| 9:K:1019:ARG:CB     | 9:K:1059:ARG:HH11    | 2.24                     | 0.49              |
| 9:K:1091:ALA:C      | 9:K:1093:SER:H       | 2.21                     | 0.49              |
| 9:K8:798:LEU:HB2    | 9:K8:842:ILE:HD11    | 1.93                     | 0.49              |
| 10:C24:33:ILE:HG22  | 10:C24:158:LEU:HD22  | 1.93                     | 0.49              |
| 10:C24:966:CYS:HA   | 10:C24:1025:LEU:HD13 | 1.93                     | 0.49              |
| 10:C24:1271:PHE:HD1 | 10:C24:1273:GLY:H    | 1.54                     | 0.49              |
| 11:A40:72:ILE:HD11  | 21:H16:348:ALA:HA    | 1.94                     | 0.49              |
| 11:A40:362:ARG:CD   | 11:A40:366:ARG:CZ    | 2.87                     | 0.49              |
| 12:A:403:MET:HA     | 12:A:406:MET:HE3     | 1.93                     | 0.49              |
| 13:V:909:ALA:CB     | 15:J:703:LEU:HD21    | 2.41                     | 0.49              |
| 10:C:667:ILE:HG12   | 10:C:670:GLU:CA      | 2.43                     | 0.49              |
| 10:C:855:VAL:HB     | 10:C:856:PRO:HD3     | 1.94                     | 0.49              |
| 10:C:1111:SER:OG    | 10:C:1114:TYR:HD2    | 1.94                     | 0.49              |
| 10:C:1163:LEU:CB    | 10:C:1166:SER:OG     | 2.60                     | 0.49              |
| 10:C8:1258:LEU:CA   | 10:C8:1323:LEU:CD1   | 2.90                     | 0.49              |
| 10:C8:1293:THR:CG2  | 10:C8:1369:LEU:HD13  | 2.42                     | 0.49              |
| 11:A16:51:THR:CG2   | 22:I:317:HIS:HB2     | 2.42                     | 0.49              |
| 18:B:254:LEU:O      | 18:B:256:VAL:HG23    | 2.13                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B:1532:PHE:HB3   | 18:B:1533:PRO:HD3   | 1.94                     | 0.49              |
| 18:B:1753:PRO:HG3   | 18:B:1762:CYS:SG    | 2.52                     | 0.49              |
| 18:B8:90:ILE:HD11   | 18:B8:131:ILE:CD1   | 2.42                     | 0.49              |
| 18:B8:119:VAL:O     | 18:B8:119:VAL:HG12  | 2.11                     | 0.49              |
| 18:B8:154:LEU:HD22  | 18:B8:224:GLU:CD    | 2.36                     | 0.49              |
| 18:B8:463:SER:O     | 18:B8:467:ILE:HG12  | 2.11                     | 0.49              |
| 18:B8:690:TRP:CH2   | 18:B8:787:VAL:CG2   | 2.94                     | 0.49              |
| 18:B8:932:THR:HA    | 18:B8:998:LEU:CD1   | 2.43                     | 0.49              |
| 18:B8:1123:ASN:O    | 18:B8:1124:GLY:C    | 2.49                     | 0.49              |
| 18:B8:1684:TRP:CH2  | 18:B8:1752:PRO:CG   | 2.95                     | 0.49              |
| 19:48:232:TYR:CD2   | 19:48:233:ASP:OD1   | 2.65                     | 0.49              |
| 21:H24:284:LEU:HD21 | 23:J24:647:MET:O    | 2.13                     | 0.49              |
| 24:D:387:LEU:CB     | 24:D16:746:ALA:CB   | 2.82                     | 0.49              |
| 24:D40:436:LEU:HD11 | 24:D40:472:ILE:HD12 | 1.94                     | 0.49              |
| 10:C32:277:SER:O    | 10:C32:280:SER:N    | 2.36                     | 0.49              |
| 10:C32:300:VAL:CG1  | 10:C32:317:ARG:CG   | 2.88                     | 0.49              |
| 12:A48:362:ARG:CG   | 12:A48:366:ARG:NH2  | 2.75                     | 0.49              |
| 1:R:1381:GLU:C      | 1:R:1382:LYS:HG3    | 2.36                     | 0.49              |
| 3:N:177:TYR:HB2     | 3:N:193:LEU:HB3     | 1.93                     | 0.49              |
| 1:R8:1194:ARG:O     | 1:R8:1195:ARG:C     | 2.52                     | 0.49              |
| 1:R16:1223:PHE:CZ   | 5:P16:676:GLN:NE2   | 2.78                     | 0.49              |
| 2:M16:544:LEU:HD11  | 2:M16:586:ALA:CB    | 2.43                     | 0.49              |
| 5:P:109:ILE:HG23    | 14:W:18:PRO:CG      | 2.35                     | 0.49              |
| 5:P:187:TRP:CZ3     | 5:P:191:ARG:CG      | 2.95                     | 0.49              |
| 5:P16:285:PRO:HG2   | 5:P16:310:ARG:HA    | 1.95                     | 0.49              |
| 5:P16:607:PHE:HB2   | 5:P16:629:ARG:NH1   | 2.28                     | 0.49              |
| 6:O16:105:ASN:ND2   | 6:O16:134:ARG:NH2   | 2.59                     | 0.49              |
| 9:K:1093:SER:O      | 9:K:1097:VAL:HG23   | 2.12                     | 0.49              |
| 9:K8:1142:ARG:HH21  | 9:K8:1204:THR:C     | 2.19                     | 0.49              |
| 10:C16:1167:PHE:C   | 10:C16:1169:ASN:N   | 2.70                     | 0.49              |
| 10:C16:1693:LYS:CE  | 10:C16:1749:ASP:OD1 | 2.60                     | 0.49              |
| 11:A24:388:VAL:CG2  | 11:A24:459:ARG:HH22 | 2.25                     | 0.49              |
| 11:A24:587:VAL:HG22 | 11:A24:627:ILE:HD13 | 1.95                     | 0.49              |
| 10:C24:1163:LEU:CB  | 10:C24:1166:SER:OG  | 2.60                     | 0.49              |
| 10:C24:1394:GLN:CD  | 24:D24:1158:SER:HB2 | 2.38                     | 0.49              |
| 11:A40:505:PRO:HG3  | 11:A40:520:HIS:HD2  | 1.78                     | 0.49              |
| 14:W:646:ALA:N      | 14:W:647:PRO:HD2    | 2.28                     | 0.49              |
| 10:C:153:ALA:CA     | 24:D:1403:LEU:HD11  | 2.42                     | 0.49              |
| 10:C:281:ASP:CG     | 24:D:1398:ARG:CD    | 2.86                     | 0.49              |
| 10:C:754:MET:CE     | 10:C:819:GLN:HB3    | 2.42                     | 0.49              |
| 10:C8:265:PHE:HE1   | 10:C8:389:LEU:HD12  | 1.76                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:C8:1624:LEU:HD23 | 10:C8:1628:SER:CB  | 2.38                     | 0.49              |
| 11:A16:154:ILE:HG23 | 18:B:1851:VAL:HG21 | 1.95                     | 0.49              |
| 11:A16:445:ASN:ND2  | 17:F8:65:ARG:NH1   | 2.59                     | 0.49              |
| 11:A32:310:GLY:HA3  | 11:A32:313:GLN:OE1 | 2.12                     | 0.49              |
| 11:A32:643:SER:O    | 11:A32:659:ARG:HD2 | 2.12                     | 0.49              |
| 18:B8:243:GLY:HA2   | 18:B8:248:SER:OG   | 2.13                     | 0.49              |
| 18:B8:424:SER:O     | 18:B8:428:GLN:HB2  | 2.12                     | 0.49              |
| 18:B8:1065:LYS:C    | 18:B8:1067:SER:N   | 2.71                     | 0.49              |
| 18:B8:1276:LYS:HG2  | 18:B8:1291:LEU:O   | 2.13                     | 0.49              |
| 19:4:362:ALA:HB3    | 19:4:417:ASP:OD2   | 2.12                     | 0.49              |
| 20:E:438:SER:O      | 20:E:440:VAL:N     | 2.43                     | 0.49              |
| 20:E8:11:VAL:HG21   | 20:E8:278:GLU:HG3  | 1.94                     | 0.49              |
| 20:E8:480:MET:CE    | 20:E8:493:TRP:CE3  | 2.95                     | 0.49              |
| 21:H:154:VAL:HG11   | 21:H:188:ARG:HE    | 1.77                     | 0.49              |
| 22:I:199:PHE:CG     | 23:J32:620:MET:HG3 | 2.44                     | 0.49              |
| 22:I:203:GLN:OE1    | 22:I:209:TRP:HZ2   | 1.96                     | 0.49              |
| 22:I:328:TYR:CE1    | 23:J32:717:ILE:CG2 | 2.95                     | 0.49              |
| 21:H24:322:LEU:HD22 | 22:I24:300:LEU:CD1 | 2.43                     | 0.49              |
| 21:H16:154:VAL:HG11 | 21:H16:188:ARG:HE  | 1.77                     | 0.49              |
| 22:I16:328:TYR:CE1  | 23:J16:717:ILE:CG2 | 2.95                     | 0.49              |
| 24:D:1452:LYS:HE2   | 24:D:1456:GLU:OE1  | 2.11                     | 0.49              |
| 24:D8:1328:ASN:HD21 | 24:D16:729:LEU:CD2 | 2.26                     | 0.49              |
| 24:D16:552:VAL:HG21 | 24:D16:592:ILE:CD1 | 2.42                     | 0.49              |
| 24:D24:552:VAL:HG21 | 24:D24:592:ILE:CD1 | 2.42                     | 0.49              |
| 10:C32:386:ASN:O    | 10:C32:390:HIS:HD2 | 1.90                     | 0.49              |
| 1:R:983:ARG:CD      | 24:D:1364:PRO:O    | 2.58                     | 0.49              |
| 1:R:1033:LYS:NZ     | 24:D:1432:THR:OG1  | 2.19                     | 0.49              |
| 1:R:1123:ASN:OD1    | 2:M:834:ASP:HB3    | 2.12                     | 0.49              |
| 2:M:403:LEU:CD2     | 2:M:425:ALA:HB3    | 2.40                     | 0.49              |
| 2:M:519:TYR:CD2     | 2:M:520:ILE:HG13   | 2.47                     | 0.49              |
| 2:M:625:HIS:NE2     | 3:N:225:PRO:CB     | 2.76                     | 0.49              |
| 2:M:651:ARG:HG3     | 2:M:664:MET:CE     | 2.42                     | 0.49              |
| 2:M8:519:TYR:CD2    | 2:M8:520:ILE:HG13  | 2.47                     | 0.49              |
| 2:M16:420:CYS:SG    | 8:L16:391:TRP:CH2  | 3.06                     | 0.49              |
| 2:M16:519:TYR:CD2   | 2:M16:520:ILE:HG13 | 2.47                     | 0.49              |
| 3:N16:2:PRO:C       | 3:N16:3:GLY:O      | 2.56                     | 0.49              |
| 6:O:303:MET:HE1     | 6:O:322:GLU:HG3    | 1.95                     | 0.49              |
| 7:Q:290:ASP:OD2     | 7:Q:293:THR:OG1    | 2.27                     | 0.49              |
| 5:P8:187:TRP:CZ3    | 5:P8:191:ARG:CG    | 2.95                     | 0.49              |
| 5:P8:285:PRO:HG2    | 5:P8:310:ARG:HA    | 1.95                     | 0.49              |
| 5:P8:479:ALA:N      | 5:P8:480:PRO:CD    | 2.75                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:O8:23:ARG:NH2      | 6:O8:37:GLU:OE1      | 2.46                     | 0.49              |
| 6:O16:23:ARG:NH2     | 6:O16:37:GLU:OE1     | 2.46                     | 0.49              |
| 7:Q16:33:ARG:HH22    | 7:Q16:345:ASP:HB3    | 1.77                     | 0.49              |
| 8:L:1092:LEU:HD11    | 9:K:999:PHE:HD2      | 1.76                     | 0.49              |
| 10:C16:1111:SER:OG   | 10:C16:1114:TYR:HD2  | 1.94                     | 0.49              |
| 11:A24:28:SER:C      | 11:A24:30:PHE:N      | 2.70                     | 0.49              |
| 11:A24:36:ASN:OD1    | 11:A24:39:GLN:HG3    | 2.13                     | 0.49              |
| 10:C24:420:TYR:CZ    | 10:C24:435:SER:HB3   | 2.48                     | 0.49              |
| 10:C24:1017:HIS:NE2  | 10:C24:1139:ARG:HD3  | 2.27                     | 0.49              |
| 10:C24:1285:VAL:HG21 | 10:C24:1738:MET:HE2  | 0.51                     | 0.49              |
| 10:C24:1624:LEU:CD2  | 10:C24:1632:LEU:HD11 | 2.41                     | 0.49              |
| 11:A40:1:MET:C       | 11:A40:3:ASN:N       | 2.71                     | 0.49              |
| 11:A40:28:SER:C      | 11:A40:30:PHE:N      | 2.70                     | 0.49              |
| 11:A40:445:ASN:ND2   | 17:F16:65:ARG:NH1    | 2.59                     | 0.49              |
| 10:C:705:TYR:O       | 10:C:794:LYS:NZ      | 2.44                     | 0.49              |
| 10:C:1023:LEU:CA     | 10:C:1210:ILE:HD11   | 2.42                     | 0.49              |
| 10:C8:26:ARG:CZ      | 10:C8:148:GLU:OE2    | 2.60                     | 0.49              |
| 10:C8:951:PRO:HA     | 10:C8:958:PHE:HE2    | 1.77                     | 0.49              |
| 10:C8:1352:GLN:NE2   | 10:C8:1357:LEU:CD1   | 2.74                     | 0.49              |
| 10:C8:1624:LEU:CD2   | 10:C8:1632:LEU:HD11  | 2.41                     | 0.49              |
| 11:A16:388:VAL:CB    | 11:A16:459:ARG:HH12  | 2.26                     | 0.49              |
| 11:A32:124:ASN:HA    | 18:B8:1523:ARG:HH11  | 1.77                     | 0.49              |
| 11:A32:198:PRO:CB    | 11:A32:200:HIS:HE1   | 2.24                     | 0.49              |
| 18:B:1065:LYS:C      | 18:B:1067:SER:N      | 2.71                     | 0.49              |
| 18:B:1590:LEU:HA     | 18:B:1593:PHE:CD2    | 2.48                     | 0.49              |
| 18:B8:712:PRO:HG3    | 18:B8:759:MET:HE2    | 1.84                     | 0.49              |
| 19:4:185:GLY:C       | 19:4:187:SER:H       | 2.19                     | 0.49              |
| 19:48:103:GLN:CD     | 19:48:411:LEU:CD1    | 2.81                     | 0.49              |
| 22:I:131:ARG:CG      | 23:J32:557:ARG:CZ    | 2.64                     | 0.49              |
| 21:H24:154:VAL:HG11  | 21:H24:188:ARG:HE    | 1.77                     | 0.49              |
| 21:H16:322:LEU:HD22  | 22:I16:300:LEU:CD1   | 2.42                     | 0.49              |
| 22:I16:178:LEU:HD12  | 23:J16:599:LEU:HD22  | 1.95                     | 0.49              |
| 10:C32:520:TYR:OH    | 10:C32:542:ASP:OD2   | 2.23                     | 0.49              |
| 10:C32:1283:LEU:CD1  | 10:C32:1357:LEU:HD11 | 2.40                     | 0.49              |
| 10:C32:1549:VAL:O    | 10:C32:1553:VAL:HG23 | 2.13                     | 0.49              |
| 10:C32:1708:ARG:HH21 | 10:C32:1733:ARG:NH2  | 2.10                     | 0.49              |
| 1:R:1139:ARG:CD      | 1:R:1157:ARG:HH22    | 2.11                     | 0.49              |
| 1:R:1334:GLU:CB      | 10:C:1170:VAL:HG23   | 2.42                     | 0.49              |
| 2:M:339:GLU:O        | 2:M:341:ASP:N        | 2.44                     | 0.49              |
| 2:M:584:VAL:HG12     | 2:M:584:VAL:O        | 2.13                     | 0.49              |
| 2:M16:625:HIS:NE2    | 3:N16:225:PRO:CB     | 2.76                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 3:N16:29:ALA:HB2     | 3:N16:62:VAL:HG13    | 1.94                     | 0.49              |
| 5:P8:543:GLY:HA2     | 5:P8:587:LEU:HD13    | 1.94                     | 0.49              |
| 5:P16:247:GLU:N      | 5:P16:247:GLU:CD     | 2.70                     | 0.49              |
| 6:O16:23:ARG:CZ      | 6:O16:37:GLU:OE1     | 2.61                     | 0.49              |
| 6:O16:42:SER:HB2     | 7:Q16:40:TYR:OH      | 2.12                     | 0.49              |
| 8:L16:1089:MET:HE3   | 9:K16:1000:SER:HB2   | 1.95                     | 0.49              |
| 9:K8:806:LEU:CD1     | 9:K8:874:VAL:HG12    | 2.37                     | 0.49              |
| 9:K8:1048:GLN:HB3    | 9:K8:1049:ASP:H      | 1.55                     | 0.49              |
| 10:C16:1033:GLY:C    | 10:C16:1218:ARG:NH2  | 2.70                     | 0.49              |
| 10:C24:1659:ASP:O    | 10:C24:1661:LEU:N    | 2.46                     | 0.49              |
| 14:W:598:ILE:CD1     | 14:W:626:LEU:HD23    | 2.42                     | 0.49              |
| 10:C:1161:PHE:O      | 10:C:1162:PRO:C      | 2.55                     | 0.49              |
| 10:C:1166:SER:C      | 10:C:1168:PRO:N      | 2.70                     | 0.49              |
| 10:C:1693:LYS:CE     | 10:C:1749:ASP:OD1    | 2.60                     | 0.49              |
| 10:C8:420:TYR:CZ     | 10:C8:435:SER:HB3    | 2.48                     | 0.49              |
| 10:C8:1163:LEU:CB    | 10:C8:1166:SER:OG    | 2.60                     | 0.49              |
| 10:C8:1251:PHE:HZ    | 10:C8:1319:ARG:HH12  | 1.39                     | 0.49              |
| 11:A16:48:LYS:HE3    | 22:I:313:ASP:OD2     | 2.12                     | 0.49              |
| 11:A32:88:THR:CG2    | 22:I24:301:LEU:HD21  | 2.43                     | 0.49              |
| 11:A32:288:HIS:CB    | 11:A32:354:ARG:NH1   | 2.71                     | 0.49              |
| 11:A32:322:ARG:NH1   | 11:A32:351:PHE:HZ    | 2.10                     | 0.49              |
| 11:A32:388:VAL:CB    | 11:A32:459:ARG:HH12  | 2.26                     | 0.49              |
| 11:A32:471:ASN:O     | 11:A32:473:GLY:N     | 2.45                     | 0.49              |
| 18:B:1175:ALA:CB     | 18:B:1325:MET:HE2    | 2.42                     | 0.49              |
| 19:4:86:LYS:O        | 19:4:90:GLN:HB2      | 2.13                     | 0.49              |
| 19:4:329:SER:OG      | 19:4:333:SER:HB3     | 2.12                     | 0.49              |
| 20:E:344:PRO:HG3     | 24:D:152:GLU:OE1     | 2.13                     | 0.49              |
| 21:H8:284:LEU:HD21   | 23:J8:647:MET:O      | 2.13                     | 0.49              |
| 21:H16:284:LEU:HD21  | 23:J16:647:MET:O     | 2.13                     | 0.49              |
| 21:H16:338:MET:HE3   | 23:J16:692:VAL:CG2   | 2.38                     | 0.49              |
| 24:D8:607:ALA:CB     | 24:D8:715:ARG:HH21   | 2.26                     | 0.49              |
| 24:D16:274:MET:CE    | 24:D16:321:SER:HB2   | 2.40                     | 0.49              |
| 24:D24:1428:ASN:ND2  | 24:D32:968:ILE:HD11  | 2.28                     | 0.49              |
| 24:D24:1452:LYS:HE2  | 24:D24:1456:GLU:OE1  | 2.11                     | 0.49              |
| 24:D32:274:MET:CE    | 24:D32:321:SER:HB2   | 2.40                     | 0.49              |
| 10:C32:1002:LEU:HD23 | 10:C32:1012:ARG:NH1  | 2.26                     | 0.49              |
| 10:C32:1591:LYS:NZ   | 12:A48:139:ASP:OD2   | 2.34                     | 0.49              |
| 10:C32:1682:VAL:HG22 | 10:C32:1758:LEU:HD23 | 1.90                     | 0.49              |
| 2:M:567:ASP:OD1      | 2:M:568:PRO:HD2      | 2.12                     | 0.49              |
| 2:M8:346:VAL:C       | 2:M8:348:GLU:H       | 2.19                     | 0.49              |
| 1:R16:1139:ARG:CG    | 1:R16:1157:ARG:CZ    | 2.90                     | 0.49              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 2:M16:231:ARG:NE    | 2:M16:299:GLY:C      | 2.70                     | 0.49              |
| 2:M16:486:MET:HG3   | 2:M16:499:ILE:HD13   | 1.94                     | 0.49              |
| 3:N16:178:LYS:HE2   | 3:N16:192:LYS:HD2    | 1.95                     | 0.49              |
| 4:T16:228:ALA:HB2   | 4:T16:263:LYS:HE2    | 1.95                     | 0.49              |
| 5:P:479:ALA:N       | 5:P:480:PRO:CD       | 2.75                     | 0.49              |
| 5:P8:16:PHE:HD1     | 6:O8:311:LEU:HD12    | 1.75                     | 0.49              |
| 6:O8:103:MET:CE     | 6:O8:124:MET:HE1     | 2.39                     | 0.49              |
| 5:P16:217:PHE:CE1   | 5:P16:221:LEU:HD11   | 2.46                     | 0.49              |
| 9:K:1249:MET:HG2    | 9:K:1254:PHE:CZ      | 2.47                     | 0.49              |
| 9:K8:845:PHE:CE1    | 9:K8:849:LEU:HD11    | 2.48                     | 0.49              |
| 9:K8:994:TYR:CE2    | 9:K8:1023:LEU:HD11   | 2.48                     | 0.49              |
| 9:K8:1110:GLN:NE2   | 9:K8:1127:PHE:H      | 2.11                     | 0.49              |
| 9:K8:1122:ALA:HB1   | 9:K8:1127:PHE:HZ     | 1.77                     | 0.49              |
| 9:K8:1232:LEU:CD2   | 9:K8:1265:ILE:HG21   | 2.30                     | 0.49              |
| 9:K16:1110:GLN:HE22 | 9:K16:1126:LEU:HA    | 1.76                     | 0.49              |
| 10:C16:420:TYR:CZ   | 10:C16:435:SER:HB3   | 2.48                     | 0.49              |
| 10:C16:667:ILE:HG12 | 10:C16:670:GLU:CA    | 2.43                     | 0.49              |
| 10:C16:1250:ALA:CB  | 10:C16:1309:ARG:HH11 | 2.23                     | 0.49              |
| 11:A24:1:MET:C      | 11:A24:3:ASN:N       | 2.71                     | 0.49              |
| 11:A24:445:ASN:ND2  | 17:F:65:ARG:NH1      | 2.59                     | 0.49              |
| 10:C24:717:GLU:O    | 10:C24:718:HIS:C     | 2.41                     | 0.49              |
| 10:C24:764:ILE:CD1  | 10:C24:781:VAL:CG2   | 2.86                     | 0.49              |
| 10:C24:1167:PHE:C   | 10:C24:1169:ASN:N    | 2.70                     | 0.49              |
| 10:C24:1220:SER:HA  | 10:C24:1225:ARG:NH2  | 2.28                     | 0.49              |
| 11:A40:72:ILE:HD13  | 21:H16:348:ALA:HA    | 1.95                     | 0.49              |
| 11:A40:103:GLU:OE2  | 21:H16:323:TYR:CE2   | 2.66                     | 0.49              |
| 11:A40:388:VAL:CG2  | 11:A40:459:ARG:HH22  | 2.26                     | 0.49              |
| 11:A40:471:ASN:O    | 11:A40:473:GLY:N     | 2.46                     | 0.49              |
| 12:A:388:VAL:CG2    | 12:A:459:ARG:HH22    | 2.26                     | 0.49              |
| 12:A:471:ASN:O      | 12:A:473:GLY:N       | 2.46                     | 0.49              |
| 14:W:515:CYS:HB2    | 14:W:604:PRO:N       | 2.21                     | 0.49              |
| 10:C:1335:ILE:O     | 10:C:1336:ALA:C      | 2.48                     | 0.49              |
| 10:C:1424:GLN:HE21  | 10:C:1478:VAL:HG13   | 1.72                     | 0.49              |
| 10:C8:556:VAL:CG1   | 10:C8:565:ARG:NH1    | 2.75                     | 0.49              |
| 10:C8:754:MET:CE    | 10:C8:819:GLN:HB3    | 2.42                     | 0.49              |
| 11:A16:47:LEU:HD12  | 23:J32:700:LEU:HD11  | 1.93                     | 0.49              |
| 11:A16:310:GLY:HA3  | 11:A16:313:GLN:OE1   | 2.12                     | 0.49              |
| 11:A16:778:ILE:HD13 | 11:A16:816:ALA:HB2   | 1.95                     | 0.49              |
| 11:A32:1:MET:C      | 11:A32:3:ASN:N       | 2.71                     | 0.49              |
| 18:B:932:THR:HA     | 18:B:998:LEU:CD1     | 2.43                     | 0.49              |
| 18:B:1133:THR:C     | 18:B:1135:ASP:H      | 2.21                     | 0.49              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B8:1045:LYS:HZ3  | 18:B8:1100:LEU:CD2   | 2.17                     | 0.49              |
| 18:B8:1419:LYS:CG   | 18:B8:1468:PHE:HE1   | 2.17                     | 0.49              |
| 18:B8:1532:PHE:HB3  | 18:B8:1533:PRO:HD3   | 1.94                     | 0.49              |
| 20:E:448:LYS:O      | 20:E:451:ILE:HB      | 2.13                     | 0.49              |
| 19:48:111:LYS:HE2   | 20:E8:517:PHE:CD2    | 2.47                     | 0.49              |
| 19:48:339:LEU:HD23  | 24:D8:140:ALA:HB2    | 1.95                     | 0.49              |
| 10:C32:182:ASP:CB   | 10:C32:183:PRO:CD    | 2.84                     | 0.49              |
| 1:R:1326:GLY:H      | 10:C:1154:TRP:NE1    | 2.11                     | 0.49              |
| 2:M8:625:HIS:HE2    | 3:N8:225:PRO:CA      | 2.26                     | 0.49              |
| 2:M8:730:GLU:OE1    | 8:L16:504:GLN:NE2    | 2.46                     | 0.49              |
| 3:N8:26:ILE:HD11    | 3:N8:40:VAL:HG21     | 1.95                     | 0.49              |
| 1:R16:1124:TRP:HZ2  | 4:T16:669:PRO:CD     | 2.24                     | 0.49              |
| 4:T8:228:ALA:HB2    | 4:T8:263:LYS:HE2     | 1.95                     | 0.49              |
| 5:P:188:LEU:HD23    | 5:P:380:MET:CE       | 2.35                     | 0.49              |
| 7:Q8:181:ALA:HB3    | 7:Q8:198:TYR:CD2     | 2.48                     | 0.49              |
| 7:Q8:279:LEU:HG     | 7:Q8:313:ILE:HG21    | 1.94                     | 0.49              |
| 5:P16:187:TRP:CZ3   | 5:P16:191:ARG:CG     | 2.96                     | 0.49              |
| 9:K:908:PHE:HB3     | 9:K:957:ILE:HG12     | 1.95                     | 0.49              |
| 9:K8:1074:ARG:CD    | 9:K8:1126:LEU:HD22   | 2.43                     | 0.49              |
| 10:C16:412:MET:O    | 10:C16:416:VAL:HG23  | 2.13                     | 0.49              |
| 10:C16:951:PRO:HA   | 10:C16:958:PHE:HE2   | 1.77                     | 0.49              |
| 10:C16:1078:GLY:O   | 10:C16:1080:SER:N    | 2.46                     | 0.49              |
| 10:C16:1624:LEU:CD2 | 10:C16:1632:LEU:HD11 | 2.41                     | 0.49              |
| 10:C24:667:ILE:HG12 | 10:C24:670:GLU:CA    | 2.43                     | 0.49              |
| 10:C24:1033:GLY:C   | 10:C24:1218:ARG:NH2  | 2.70                     | 0.49              |
| 10:C24:1293:THR:CG2 | 10:C24:1369:LEU:HD13 | 2.42                     | 0.49              |
| 10:C24:1335:ILE:O   | 10:C24:1336:ALA:C    | 2.48                     | 0.49              |
| 11:A40:587:VAL:HG21 | 11:A40:636:PHE:CE1   | 2.41                     | 0.49              |
| 11:A40:643:SER:O    | 11:A40:659:ARG:HD2   | 2.12                     | 0.49              |
| 10:C:26:ARG:CZ      | 10:C:148:GLU:OE2     | 2.60                     | 0.49              |
| 10:C:1002:LEU:HD23  | 10:C:1012:ARG:NH1    | 2.26                     | 0.49              |
| 10:C8:960:PHE:HZ    | 10:C8:1138:GLU:OE1   | 1.90                     | 0.49              |
| 11:A16:1:MET:C      | 11:A16:3:ASN:N       | 2.71                     | 0.49              |
| 11:A16:88:THR:CG2   | 22:I:301:LEU:HD21    | 2.43                     | 0.49              |
| 11:A32:778:ILE:HD13 | 11:A32:816:ALA:HB2   | 1.95                     | 0.49              |
| 18:B:1543:HIS:O     | 18:B:1547:GLN:HG2    | 2.12                     | 0.49              |
| 18:B8:7:VAL:HG12    | 18:B8:8:ASP:H        | 1.76                     | 0.49              |
| 18:B8:789:LEU:CD2   | 18:B8:793:LEU:CD1    | 2.85                     | 0.49              |
| 18:B8:1590:LEU:HA   | 18:B8:1593:PHE:CD2   | 2.48                     | 0.49              |
| 19:48:104:GLY:H     | 19:48:117:ILE:HD12   | 1.78                     | 0.49              |
| 21:H8:149:HIS:CD2   | 23:J8:565:ALA:HB3    | 2.48                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A48:471:ASN:O    | 12:A48:473:GLY:N    | 2.46                     | 0.49              |
| 3:N:178:LYS:HE2     | 3:N:192:LYS:HD2     | 1.95                     | 0.49              |
| 1:R8:1123:ASN:OD1   | 2:M8:834:ASP:HB3    | 2.12                     | 0.49              |
| 1:R8:1466:LYS:HG2   | 6:O8:160:LEU:HD21   | 1.87                     | 0.49              |
| 2:M8:428:SER:HB2    | 8:L8:355:SER:CB     | 2.32                     | 0.49              |
| 1:R16:1266:THR:OG1  | 5:P16:684:ARG:NH2   | 2.45                     | 0.49              |
| 5:P:401:ARG:NH2     | 5:P:404:ILE:HB      | 2.28                     | 0.49              |
| 7:Q:181:ALA:HB3     | 7:Q:198:TYR:CD2     | 2.48                     | 0.49              |
| 6:O8:288:TRP:CZ3    | 6:O8:315:TRP:HH2    | 2.31                     | 0.49              |
| 8:L8:608:PHE:O      | 8:L8:639:ARG:NH2    | 2.45                     | 0.49              |
| 9:K:840:TRP:CH2     | 9:K:907:ILE:HG13    | 2.48                     | 0.49              |
| 9:K:1180:TRP:CZ2    | 9:K:1206:LEU:CD1    | 2.92                     | 0.49              |
| 10:C16:297:GLN:OE1  | 10:C16:320:TRP:NE1  | 2.37                     | 0.49              |
| 10:C16:1163:LEU:CB  | 10:C16:1166:SER:OG  | 2.60                     | 0.49              |
| 11:A24:48:LYS:HE3   | 22:I8:313:ASP:OD2   | 2.12                     | 0.49              |
| 11:A24:88:THR:CG2   | 22:I8:301:LEU:HD21  | 2.43                     | 0.49              |
| 11:A24:322:ARG:NH1  | 11:A24:351:PHE:HZ   | 2.11                     | 0.49              |
| 10:C24:898:GLN:HE22 | 10:C24:1138:GLU:CD  | 2.21                     | 0.49              |
| 10:C24:951:PRO:HA   | 10:C24:958:PHE:HE2  | 1.77                     | 0.49              |
| 10:C24:1547:LYS:HZ3 | 24:D24:1405:GLY:C   | 2.20                     | 0.49              |
| 12:A:310:GLY:HA3    | 12:A:313:GLN:OE1    | 2.12                     | 0.49              |
| 12:A:362:ARG:CG     | 12:A:366:ARG:NH2    | 2.75                     | 0.49              |
| 12:A:388:VAL:CB     | 12:A:459:ARG:HH12   | 2.26                     | 0.49              |
| 12:A:558:SER:C      | 12:A:560:MET:N      | 2.70                     | 0.49              |
| 10:C:758:GLN:HE21   | 10:C:819:GLN:CG     | 2.24                     | 0.49              |
| 10:C:1220:SER:HA    | 10:C:1225:ARG:NH2   | 2.28                     | 0.49              |
| 10:C8:168:ARG:HH12  | 10:C8:229:PRO:HA    | 1.70                     | 0.49              |
| 11:A16:198:PRO:CB   | 11:A16:200:HIS:HE1  | 2.24                     | 0.49              |
| 11:A16:505:PRO:HG3  | 11:A16:520:HIS:HD2  | 1.78                     | 0.49              |
| 11:A32:51:THR:CG2   | 22:I24:317:HIS:HB2  | 2.42                     | 0.49              |
| 18:B:1684:TRP:CZ2   | 18:B:1752:PRO:HG3   | 2.48                     | 0.49              |
| 18:B8:109:MET:HE1   | 18:B8:120:ALA:HB2   | 1.94                     | 0.49              |
| 18:B8:202:LEU:HD12  | 18:B8:820:ARG:HH11  | 1.77                     | 0.49              |
| 18:B8:1101:TYR:CE1  | 18:B8:1105:LEU:CD1  | 2.93                     | 0.49              |
| 19:4:104:GLY:H      | 19:4:117:ILE:HD12   | 1.78                     | 0.49              |
| 20:E:11:VAL:HG21    | 20:E:278:GLU:HG3    | 1.94                     | 0.49              |
| 21:H:239:SER:HB3    | 23:J32:603:LEU:HD21 | 1.93                     | 0.49              |
| 22:I8:328:TYR:CE1   | 23:J8:717:ILE:CG2   | 2.95                     | 0.49              |
| 21:H16:215:ARG:NH1  | 21:H16:219:LYS:NZ   | 2.61                     | 0.49              |
| 24:D24:607:ALA:CB   | 24:D24:715:ARG:HH21 | 2.26                     | 0.49              |
| 24:D32:607:ALA:CB   | 24:D32:715:ARG:HH21 | 2.26                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C32:1078:GLY:O   | 10:C32:1080:SER:N   | 2.46                     | 0.49              |
| 10:C32:1166:SER:C   | 10:C32:1168:PRO:N   | 2.70                     | 0.49              |
| 10:C32:1760:GLU:OE2 | 12:A48:140:TRP:NE1  | 2.44                     | 0.49              |
| 2:M:428:SER:OG      | 8:L:355:SER:OG      | 2.01                     | 0.48              |
| 3:N:163:ALA:O       | 3:N:164:PRO:C       | 2.51                     | 0.48              |
| 3:N:167:LEU:HD23    | 3:N:169:SER:HB2     | 1.95                     | 0.48              |
| 2:M8:200:THR:HG21   | 3:N8:14:VAL:HB      | 1.95                     | 0.48              |
| 3:N8:116:ILE:HG23   | 3:N8:177:TYR:CZ     | 2.47                     | 0.48              |
| 1:R16:1123:ASN:OD1  | 2:M16:834:ASP:HB3   | 2.12                     | 0.48              |
| 2:M16:820:LEU:HG    | 4:T16:656:TRP:CZ2   | 2.47                     | 0.48              |
| 4:T:167:MET:HE1     | 4:T:241:PHE:CE1     | 2.48                     | 0.48              |
| 5:P:600:PHE:CD1     | 5:P:638:SER:HB2     | 2.48                     | 0.48              |
| 6:O:23:ARG:NH2      | 6:O:37:GLU:OE1      | 2.46                     | 0.48              |
| 5:P8:167:SER:HB3    | 5:P8:398:LYS:HE3    | 1.95                     | 0.48              |
| 5:P8:233:TYR:CE1    | 5:P8:237:MET:HE2    | 2.48                     | 0.48              |
| 6:O8:288:TRP:HZ3    | 6:O8:315:TRP:HH2    | 1.59                     | 0.48              |
| 5:P16:12:GLU:C      | 5:P16:14:VAL:H      | 2.15                     | 0.48              |
| 6:O16:288:TRP:CZ3   | 6:O16:315:TRP:HH2   | 2.31                     | 0.48              |
| 6:O16:288:TRP:HZ3   | 6:O16:315:TRP:HH2   | 1.59                     | 0.48              |
| 6:O16:303:MET:HE1   | 6:O16:322:GLU:HG3   | 1.95                     | 0.48              |
| 7:Q16:181:ALA:HB3   | 7:Q16:198:TYR:CD2   | 2.48                     | 0.48              |
| 9:K:994:TYR:CE2     | 9:K:1023:LEU:HD11   | 2.48                     | 0.48              |
| 11:A24:212:LYS:NZ   | 11:A24:585:MET:HE1  | 2.10                     | 0.48              |
| 11:A40:1:MET:C      | 11:A40:3:ASN:H      | 2.20                     | 0.48              |
| 12:A:140:TRP:NE1    | 10:C:1760:GLU:OE2   | 2.44                     | 0.48              |
| 12:A:273:ARG:NE     | 12:A:479:LEU:HD23   | 2.19                     | 0.48              |
| 10:C:1078:GLY:O     | 10:C:1080:SER:N     | 2.46                     | 0.48              |
| 10:C:1133:ILE:CG1   | 10:C:1152:LYS:HD2   | 2.43                     | 0.48              |
| 10:C:1250:ALA:CB    | 10:C:1309:ARG:HH12  | 2.15                     | 0.48              |
| 10:C:1616:ILE:C     | 10:C:1618:SER:N     | 2.70                     | 0.48              |
| 10:C8:705:TYR:O     | 10:C8:794:LYS:NZ    | 2.43                     | 0.48              |
| 10:C8:1078:GLY:O    | 10:C8:1080:SER:N    | 2.46                     | 0.48              |
| 10:C8:1488:ILE:HG21 | 10:C8:1525:VAL:HG13 | 1.95                     | 0.48              |
| 11:A16:1:MET:C      | 11:A16:3:ASN:H      | 2.20                     | 0.48              |
| 11:A16:36:ASN:OD1   | 11:A16:39:GLN:HG3   | 2.13                     | 0.48              |
| 11:A32:36:ASN:OD1   | 11:A32:39:GLN:HG3   | 2.13                     | 0.48              |
| 11:A32:455:LEU:HD23 | 11:A32:458:ILE:HD12 | 1.95                     | 0.48              |
| 18:B:814:GLU:O      | 18:B:818:SER:OG     | 2.30                     | 0.48              |
| 20:E:382:HIS:HD2    | 20:E:476:PHE:CE1    | 2.30                     | 0.48              |
| 21:H:322:LEU:HD22   | 22:I:300:LEU:CD1    | 2.43                     | 0.48              |
| 21:H8:215:ARG:NH1   | 21:H8:219:LYS:NZ    | 2.61                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 21:H16:269:PHE:CE1  | 22:I16:205:ARG:CZ    | 2.90                     | 0.48              |
| 10:C32:898:GLN:HE22 | 10:C32:1138:GLU:CD   | 2.21                     | 0.48              |
| 10:C32:951:PRO:HA   | 10:C32:958:PHE:HE2   | 1.77                     | 0.48              |
| 12:A48:322:ARG:NH1  | 12:A48:351:PHE:HZ    | 2.11                     | 0.48              |
| 1:R:1369:LEU:CD1    | 6:O:211:ASN:OD1      | 2.59                     | 0.48              |
| 2:M:486:MET:HG3     | 2:M:499:ILE:HD13     | 1.94                     | 0.48              |
| 3:N:9:GLY:C         | 3:N:36:LYS:HZ1       | 2.21                     | 0.48              |
| 2:M8:625:HIS:NE2    | 3:N8:225:PRO:CB      | 2.76                     | 0.48              |
| 3:N8:9:GLY:C        | 3:N8:36:LYS:HZ1      | 2.20                     | 0.48              |
| 5:P:233:TYR:CE1     | 5:P:237:MET:HE2      | 2.48                     | 0.48              |
| 5:P:578:LEU:CD1     | 5:P:608:LYS:NZ       | 2.77                     | 0.48              |
| 6:O:175:TRP:HZ3     | 6:O:185:PRO:HB2      | 1.78                     | 0.48              |
| 5:P8:280:LEU:HB3    | 5:P8:345:MET:HE1     | 1.95                     | 0.48              |
| 5:P8:578:LEU:CD1    | 5:P8:608:LYS:NZ      | 2.77                     | 0.48              |
| 6:O8:119:ARG:NH2    | 6:O8:182:GLU:CB      | 2.76                     | 0.48              |
| 5:P16:201:ILE:HG13  | 5:P16:211:TYR:CE1    | 2.48                     | 0.48              |
| 6:O16:175:TRP:HZ3   | 6:O16:185:PRO:HB2    | 1.78                     | 0.48              |
| 8:L:1077:LEU:CD1    | 9:K:1086:VAL:CG1     | 2.85                     | 0.48              |
| 9:K:845:PHE:CE1     | 9:K:849:LEU:HD11     | 2.48                     | 0.48              |
| 10:C16:269:ILE:HG23 | 10:C16:388:TYR:CE1   | 2.49                     | 0.48              |
| 10:C24:297:GLN:OE1  | 10:C24:320:TRP:NE1   | 2.37                     | 0.48              |
| 10:C24:412:MET:O    | 10:C24:416:VAL:HG23  | 2.13                     | 0.48              |
| 10:C24:1283:LEU:CD1 | 10:C24:1357:LEU:HD11 | 2.40                     | 0.48              |
| 10:C:412:MET:O      | 10:C:416:VAL:HG23    | 2.13                     | 0.48              |
| 10:C8:556:VAL:CG1   | 10:C8:565:ARG:CZ     | 2.77                     | 0.48              |
| 10:C8:1017:HIS:NE2  | 10:C8:1139:ARG:HD3   | 2.27                     | 0.48              |
| 10:C8:1757:GLN:OE1  | 16:A8:136:LEU:HD23   | 2.11                     | 0.48              |
| 11:A16:36:ASN:HD21  | 22:I:293:LYS:HE3     | 1.75                     | 0.48              |
| 11:A16:643:SER:O    | 11:A16:659:ARG:HD2   | 2.12                     | 0.48              |
| 11:A16:714:GLY:C    | 24:D16:1398:ARG:NH2  | 2.69                     | 0.48              |
| 11:A32:48:LYS:HE3   | 22:I24:313:ASP:OD2   | 2.12                     | 0.48              |
| 11:A32:362:ARG:CG   | 11:A32:366:ARG:NH2   | 2.75                     | 0.48              |
| 11:A32:587:VAL:HG22 | 11:A32:627:ILE:HD13  | 1.95                     | 0.48              |
| 18:B:202:LEU:HD12   | 18:B:820:ARG:HH11    | 1.78                     | 0.48              |
| 18:B:243:GLY:HA2    | 18:B:248:SER:OG      | 2.13                     | 0.48              |
| 18:B:399:SER:OG     | 18:B:444:VAL:O       | 2.24                     | 0.48              |
| 18:B:990:PRO:C      | 18:B:992:TRP:N       | 2.70                     | 0.48              |
| 18:B8:1133:THR:C    | 18:B8:1135:ASP:H     | 2.21                     | 0.48              |
| 18:B8:1273:GLU:O    | 18:B8:1276:LYS:HG3   | 2.13                     | 0.48              |
| 18:B8:1684:TRP:CZ2  | 18:B8:1752:PRO:HG3   | 2.48                     | 0.48              |
| 19:4:294:SER:C      | 19:4:296:GLY:H       | 2.20                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 19:4:361:ASP:OD2    | 19:4:363:SER:OG      | 2.26                     | 0.48              |
| 19:48:14:GLU:OE2    | 19:48:439:LEU:HD22   | 2.13                     | 0.48              |
| 19:48:86:LYS:O      | 19:48:90:GLN:HB2     | 2.13                     | 0.48              |
| 20:E8:382:HIS:HD2   | 20:E8:476:PHE:CE1    | 2.30                     | 0.48              |
| 21:H24:269:PHE:CE1  | 22:I24:205:ARG:CZ    | 2.90                     | 0.48              |
| 24:D:607:ALA:CB     | 24:D:715:ARG:HH21    | 2.26                     | 0.48              |
| 24:D16:607:ALA:CB   | 24:D16:715:ARG:HH21  | 2.26                     | 0.48              |
| 10:C32:412:MET:O    | 10:C32:416:VAL:HG23  | 2.13                     | 0.48              |
| 10:C32:1163:LEU:CB  | 10:C32:1166:SER:OG   | 2.60                     | 0.48              |
| 10:C32:1757:GLN:OE1 | 12:A48:136:LEU:HD23  | 2.11                     | 0.48              |
| 12:A48:587:VAL:HG21 | 12:A48:636:PHE:CE1   | 2.41                     | 0.48              |
| 12:A48:587:VAL:HG22 | 12:A48:627:ILE:HD13  | 1.94                     | 0.48              |
| 2:M:349:ASP:C       | 2:M:351:ALA:H        | 2.09                     | 0.48              |
| 2:M8:328:THR:O      | 2:M8:329:GLU:C       | 2.53                     | 0.48              |
| 2:M8:351:ALA:HB2    | 8:L8:219:ILE:CG2     | 2.33                     | 0.48              |
| 2:M8:540:TYR:CD1    | 2:M8:555:LEU:HD22    | 2.46                     | 0.48              |
| 2:M8:783:TRP:O      | 8:L16:472:GLU:OE1    | 2.31                     | 0.48              |
| 1:R16:1420:PHE:O    | 1:R16:1423:SER:OG    | 2.32                     | 0.48              |
| 5:P:322:CYS:SG      | 13:V:763:LYS:HD3     | 2.51                     | 0.48              |
| 9:K8:788:LEU:HD22   | 9:K8:856:ILE:CD1     | 2.20                     | 0.48              |
| 9:K8:840:TRP:CH2    | 9:K8:907:ILE:HG13    | 2.48                     | 0.48              |
| 9:K8:850:LEU:HD11   | 9:K8:864:ILE:HG22    | 1.96                     | 0.48              |
| 10:C16:460:TRP:CD1  | 10:C16:495:LYS:HZ3   | 2.32                     | 0.48              |
| 10:C16:667:ILE:CB   | 10:C16:670:GLU:H     | 2.26                     | 0.48              |
| 11:A24:257:GLN:CD   | 11:A24:263:ASP:OD1   | 2.51                     | 0.48              |
| 10:C24:390:HIS:ND1  | 10:C24:452:LEU:HB3   | 2.26                     | 0.48              |
| 10:C24:758:GLN:HE21 | 10:C24:819:GLN:CG    | 2.24                     | 0.48              |
| 10:C24:1137:SER:HB3 | 10:C24:1143:LEU:HD12 | 1.96                     | 0.48              |
| 11:A40:322:ARG:NH1  | 11:A40:351:PHE:HZ    | 2.11                     | 0.48              |
| 12:A:505:PRO:HG3    | 12:A:520:HIS:HD2     | 1.78                     | 0.48              |
| 10:C:586:PRO:CD     | 10:C:650:ARG:HH12    | 2.10                     | 0.48              |
| 10:C8:1133:ILE:CG1  | 10:C8:1152:LYS:HD2   | 2.43                     | 0.48              |
| 10:C8:1220:SER:HA   | 10:C8:1225:ARG:NH2   | 2.28                     | 0.48              |
| 10:C8:1293:THR:HG23 | 10:C8:1369:LEU:HD13  | 1.96                     | 0.48              |
| 11:A32:1:MET:C      | 11:A32:3:ASN:H       | 2.20                     | 0.48              |
| 11:A32:54:ASN:CB    | 11:A32:59:GLN:HE22   | 2.21                     | 0.48              |
| 11:A32:154:ILE:HG23 | 18:B8:1851:VAL:HG21  | 1.95                     | 0.48              |
| 18:B:603:PHE:HB3    | 18:B:619:ARG:NH2     | 2.29                     | 0.48              |
| 18:B:1013:VAL:O     | 18:B:1017:THR:HG22   | 2.14                     | 0.48              |
| 18:B:1098:MET:HE2   | 18:B:1139:LYS:HA     | 1.95                     | 0.48              |
| 18:B:1273:GLU:O     | 18:B:1276:LYS:HG3    | 2.13                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B:1527:THR:O     | 18:B:1531:TRP:CD1    | 2.67                     | 0.48              |
| 18:B8:1529:GLU:OE1  | 24:D32:1411:ASN:HB3  | 2.12                     | 0.48              |
| 19:4:117:ILE:HG13   | 19:4:150:LEU:CD2     | 2.44                     | 0.48              |
| 21:H8:253:ARG:NH1   | 23:J8:614:ASP:OD1    | 2.47                     | 0.48              |
| 21:H8:322:LEU:HD22  | 22:I8:300:LEU:CD1    | 2.43                     | 0.48              |
| 24:D:436:LEU:HD11   | 24:D:472:ILE:HD12    | 1.94                     | 0.48              |
| 10:C32:1220:SER:HA  | 10:C32:1225:ARG:NH2  | 2.28                     | 0.48              |
| 10:C32:1293:THR:CG2 | 10:C32:1369:LEU:HD13 | 2.42                     | 0.48              |
| 10:C32:1616:ILE:C   | 10:C32:1618:SER:N    | 2.70                     | 0.48              |
| 12:A48:505:PRO:HG3  | 12:A48:520:HIS:HD2   | 1.78                     | 0.48              |
| 12:A48:643:SER:O    | 12:A48:659:ARG:HD2   | 2.13                     | 0.48              |
| 1:R:1418:GLU:OE2    | 6:O:159:SER:HB3      | 2.13                     | 0.48              |
| 2:M:820:LEU:HG      | 4:T:656:TRP:CZ2      | 2.48                     | 0.48              |
| 3:N:2:PRO:C         | 3:N:3:GLY:O          | 2.56                     | 0.48              |
| 5:P:12:GLU:CD       | 5:P:78:GLY:H         | 2.22                     | 0.48              |
| 5:P:394:ASN:O       | 5:P:396:SER:N        | 2.29                     | 0.48              |
| 7:Q8:10:VAL:HG21    | 7:Q8:327:LEU:CD2     | 2.43                     | 0.48              |
| 9:K:1110:GLN:HE22   | 9:K:1127:PHE:H       | 1.62                     | 0.48              |
| 9:K8:738:GLN:OE1    | 9:K8:756:ASN:HB2     | 2.13                     | 0.48              |
| 10:C16:300:VAL:CG1  | 10:C16:317:ARG:CG    | 2.88                     | 0.48              |
| 10:C16:717:GLU:O    | 10:C16:718:HIS:C     | 2.41                     | 0.48              |
| 11:A24:505:PRO:HG3  | 11:A24:520:HIS:HD2   | 1.78                     | 0.48              |
| 11:A24:778:ILE:HD13 | 11:A24:816:ALA:HB2   | 1.95                     | 0.48              |
| 10:C24:754:MET:CE   | 10:C24:819:GLN:HB3   | 2.42                     | 0.48              |
| 10:C24:1591:LYS:NZ  | 11:A40:139:ASP:OD2   | 2.34                     | 0.48              |
| 11:A40:587:VAL:HG22 | 11:A40:627:ILE:HD13  | 1.95                     | 0.48              |
| 12:A:198:PRO:CB     | 12:A:200:HIS:HE1     | 2.24                     | 0.48              |
| 12:A:778:ILE:HD13   | 12:A:816:ALA:HB2     | 1.95                     | 0.48              |
| 13:V:832:LEU:O      | 13:V:833:ASN:C       | 2.54                     | 0.48              |
| 10:C:390:HIS:CG     | 10:C:452:LEU:CB      | 2.95                     | 0.48              |
| 10:C:764:ILE:HD13   | 10:C:781:VAL:HG21    | 1.94                     | 0.48              |
| 10:C:1033:GLY:C     | 10:C:1218:ARG:NH2    | 2.70                     | 0.48              |
| 10:C:1137:SER:HB3   | 10:C:1143:LEU:HD12   | 1.96                     | 0.48              |
| 10:C:1293:THR:HG23  | 10:C:1369:LEU:HD13   | 1.96                     | 0.48              |
| 10:C:1549:VAL:O     | 10:C:1553:VAL:HG23   | 2.13                     | 0.48              |
| 10:C8:460:TRP:CD1   | 10:C8:495:LYS:HZ3    | 2.31                     | 0.48              |
| 11:A16:28:SER:C     | 11:A16:30:PHE:N      | 2.70                     | 0.48              |
| 11:A16:455:LEU:HD23 | 11:A16:458:ILE:HD12  | 1.95                     | 0.48              |
| 11:A16:471:ASN:O    | 11:A16:473:GLY:N     | 2.45                     | 0.48              |
| 11:A16:718:THR:CG2  | 24:D16:1398:ARG:NH1  | 2.61                     | 0.48              |
| 11:A32:505:PRO:HG3  | 11:A32:520:HIS:HD2   | 1.78                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:1123:ASN:O      | 18:B:1124:GLY:C      | 2.49                     | 0.48              |
| 18:B8:1013:VAL:O     | 18:B8:1017:THR:HG22  | 2.14                     | 0.48              |
| 18:B8:1102:LYS:NZ    | 18:B8:1354:ASP:CG    | 2.60                     | 0.48              |
| 18:B8:1527:THR:O     | 18:B8:1531:TRP:CD1   | 2.67                     | 0.48              |
| 18:B8:1649:SER:OG    | 18:B8:1653:LEU:HD12  | 2.14                     | 0.48              |
| 20:E:39:SER:O        | 20:E:39:SER:OG       | 2.27                     | 0.48              |
| 19:48:346:ILE:CG2    | 19:48:347:ALA:N      | 2.77                     | 0.48              |
| 20:E8:494:ILE:HD13   | 20:E8:507:LEU:HB3    | 1.94                     | 0.48              |
| 21:H:149:HIS:CD2     | 23:J32:565:ALA:HB3   | 2.48                     | 0.48              |
| 22:I24:178:LEU:HD12  | 23:J24:599:LEU:HD22  | 1.95                     | 0.48              |
| 22:I24:210:LYS:C     | 22:I16:139:GLN:HE22  | 2.20                     | 0.48              |
| 21:H16:253:ARG:NH1   | 23:J16:614:ASP:OD1   | 2.47                     | 0.48              |
| 10:C32:1285:VAL:HG21 | 10:C32:1738:MET:HE2  | 0.51                     | 0.48              |
| 1:R:979:GLN:OE1      | 24:D:1438:ALA:CA     | 2.59                     | 0.48              |
| 1:R:1449:TRP:CZ3     | 2:M:160:LEU:HD11     | 2.37                     | 0.48              |
| 2:M:335:ALA:O        | 2:M:336:SER:C        | 2.51                     | 0.48              |
| 3:N:26:ILE:HD11      | 3:N:40:VAL:HG21      | 1.95                     | 0.48              |
| 2:M16:328:THR:O      | 2:M16:329:GLU:C      | 2.53                     | 0.48              |
| 2:M16:503:TYR:CD1    | 2:M16:507:LEU:HD12   | 2.47                     | 0.48              |
| 4:T16:167:MET:HE1    | 4:T16:241:PHE:CE1    | 2.48                     | 0.48              |
| 6:O:111:LEU:HD11     | 6:O:129:SER:HA       | 1.96                     | 0.48              |
| 6:O8:60:VAL:HG22     | 6:O8:76:VAL:O        | 2.14                     | 0.48              |
| 6:O8:111:LEU:HD11    | 6:O8:129:SER:HA      | 1.96                     | 0.48              |
| 9:K8:908:PHE:HB3     | 9:K8:957:ILE:HG12    | 1.95                     | 0.48              |
| 9:K8:1093:SER:O      | 9:K8:1097:VAL:HG23   | 2.12                     | 0.48              |
| 10:C16:898:GLN:HE22  | 10:C16:1138:GLU:CD   | 2.21                     | 0.48              |
| 11:A24:471:ASN:O     | 11:A24:473:GLY:N     | 2.45                     | 0.48              |
| 11:A24:558:SER:C     | 11:A24:560:MET:N     | 2.70                     | 0.48              |
| 11:A24:743:ARG:HH22  | 24:D16:699:HIS:CD2   | 2.31                     | 0.48              |
| 10:C24:37:PHE:N      | 10:C24:38:PRO:HD2    | 2.28                     | 0.48              |
| 10:C24:855:VAL:HB    | 10:C24:856:PRO:HD3   | 1.94                     | 0.48              |
| 10:C24:1002:LEU:HD23 | 10:C24:1012:ARG:NH1  | 2.26                     | 0.48              |
| 10:C24:1250:ALA:CB   | 10:C24:1309:ARG:HH11 | 2.23                     | 0.48              |
| 10:C24:1549:VAL:O    | 10:C24:1553:VAL:HG23 | 2.13                     | 0.48              |
| 11:A40:778:ILE:HD13  | 11:A40:816:ALA:HB2   | 1.95                     | 0.48              |
| 12:A:257:GLN:CD      | 12:A:263:ASP:OD1     | 2.51                     | 0.48              |
| 12:A:305:LEU:HD12    | 12:A:317:ALA:HB2     | 1.96                     | 0.48              |
| 14:W:351:CYS:HG      | 14:W:373:TRP:CD1     | 2.31                     | 0.48              |
| 15:J:658:LEU:HA      | 15:J:661:MET:HE3     | 1.94                     | 0.48              |
| 10:C:460:TRP:CD1     | 10:C:495:LYS:HZ3     | 2.31                     | 0.48              |
| 10:C8:37:PHE:N       | 10:C8:38:PRO:HD2     | 2.28                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C8:1111:SER:OG    | 10:C8:1114:TYR:HD2   | 1.94                     | 0.48              |
| 10:C8:1166:SER:C     | 10:C8:1168:PRO:N     | 2.70                     | 0.48              |
| 17:F:72:SER:C        | 17:F:74:ILE:N        | 2.69                     | 0.48              |
| 11:A32:36:ASN:HD21   | 22:I24:293:LYS:HE3   | 1.76                     | 0.48              |
| 11:A32:388:VAL:CG2   | 11:A32:459:ARG:HH22  | 2.26                     | 0.48              |
| 18:B:113:TYR:C       | 18:B:114:GLY:O       | 2.57                     | 0.48              |
| 18:B:287:MET:HE3     | 18:B:297:GLY:HA3     | 1.95                     | 0.48              |
| 18:B:1133:THR:C      | 18:B:1135:ASP:N      | 2.72                     | 0.48              |
| 18:B8:1360:SER:O     | 18:B8:1361:ALA:C     | 2.52                     | 0.48              |
| 19:48:286:TRP:CG     | 20:E8:163:ILE:HG23   | 2.49                     | 0.48              |
| 23:J8:686:MET:SD     | 23:J8:694:ARG:CZ     | 3.01                     | 0.48              |
| 22:I16:203:GLN:OE1   | 22:I16:209:TRP:HZ2   | 1.94                     | 0.48              |
| 22:I16:368:VAL:HG22  | 23:J16:591:LYS:HD2   | 1.95                     | 0.48              |
| 24:D24:1328:ASN:HD21 | 24:D32:729:LEU:HD23  | 1.78                     | 0.48              |
| 24:D40:607:ALA:CB    | 24:D40:715:ARG:HH21  | 2.26                     | 0.48              |
| 10:C32:664:ASN:O     | 10:C32:668:ALA:N     | 2.42                     | 0.48              |
| 12:A48:388:VAL:CG2   | 12:A48:459:ARG:HH22  | 2.26                     | 0.48              |
| 1:R:1033:LYS:HG2     | 24:D:1436:ARG:NE     | 2.24                     | 0.48              |
| 3:N:26:ILE:HD12      | 3:N:40:VAL:CG2       | 2.44                     | 0.48              |
| 1:R8:1188:TYR:CE1    | 24:D40:1459:LEU:CD1  | 2.97                     | 0.48              |
| 4:T8:167:MET:HE1     | 4:T8:241:PHE:CE1     | 2.48                     | 0.48              |
| 5:P:499:TYR:CE1      | 5:P:527:LYS:HD3      | 2.49                     | 0.48              |
| 5:P:655:LEU:HD23     | 5:P:663:LEU:CD1      | 2.44                     | 0.48              |
| 6:O:173:VAL:HG22     | 6:O:189:LEU:HD12     | 1.92                     | 0.48              |
| 7:Q:10:VAL:HG21      | 7:Q:327:LEU:CD2      | 2.43                     | 0.48              |
| 7:Q:341:GLN:CG       | 10:C8:751:ARG:HH11   | 2.11                     | 0.48              |
| 5:P8:313:TRP:CZ2     | 5:P8:317:ILE:HD11    | 2.49                     | 0.48              |
| 6:O16:282:GLU:CB     | 6:O16:284:TRP:CZ2    | 2.93                     | 0.48              |
| 9:K8:1110:GLN:HE22   | 9:K8:1127:PHE:H      | 1.62                     | 0.48              |
| 10:C16:855:VAL:HB    | 10:C16:856:PRO:HD3   | 1.94                     | 0.48              |
| 11:A24:468:VAL:CG2   | 24:D16:1100:GLN:HB3  | 2.41                     | 0.48              |
| 10:C24:667:ILE:CB    | 10:C24:670:GLU:H     | 2.27                     | 0.48              |
| 10:C24:1695:LEU:CD2  | 23:J24:722:LEU:HD21  | 2.43                     | 0.48              |
| 10:C24:1812:GLU:HA   | 10:C24:1819:LEU:HD12 | 1.96                     | 0.48              |
| 12:A:587:VAL:HG21    | 12:A:636:PHE:CE1     | 2.41                     | 0.48              |
| 14:W:645:HIS:CE1     | 15:J:572:ASP:OD1     | 2.63                     | 0.48              |
| 10:C:269:ILE:HG23    | 10:C:388:TYR:CE1     | 2.49                     | 0.48              |
| 10:C:945:LEU:O       | 10:C:993:HIS:HE1     | 1.95                     | 0.48              |
| 10:C:951:PRO:HA      | 10:C:958:PHE:HE2     | 1.77                     | 0.48              |
| 10:C:1167:PHE:C      | 10:C:1169:ASN:N      | 2.70                     | 0.48              |
| 10:C:1767:LEU:CD1    | 10:C:1832:MET:HE3    | 2.44                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C8:798:VAL:HG12  | 10:C8:802:TRP:CD2    | 2.49                     | 0.48              |
| 11:A16:72:ILE:HD13  | 21:H:348:ALA:HA      | 1.95                     | 0.48              |
| 18:B:783:LYS:HE2    | 24:D16:1064:GLY:HA2  | 1.89                     | 0.48              |
| 18:B:1182:LEU:HB3   | 18:B:1202:ILE:HD13   | 1.94                     | 0.48              |
| 18:B:1276:LYS:HG2   | 18:B:1291:LEU:O      | 2.13                     | 0.48              |
| 18:B:1618:HIS:ND1   | 18:B:1622:ILE:CD1    | 2.74                     | 0.48              |
| 18:B8:746:LEU:HB2   | 18:B8:767:VAL:HG11   | 1.95                     | 0.48              |
| 18:B8:1182:LEU:HB3  | 18:B8:1202:ILE:HD13  | 1.94                     | 0.48              |
| 19:4:111:LYS:HE2    | 20:E:517:PHE:CD2     | 2.47                     | 0.48              |
| 20:E8:448:LYS:O     | 20:E8:451:ILE:HB     | 2.13                     | 0.48              |
| 22:I16:300:LEU:CG   | 23:J16:689:LEU:HD21  | 2.41                     | 0.48              |
| 23:J16:733:ALA:HA   | 23:J16:734:PRO:HD3   | 1.47                     | 0.48              |
| 10:C32:667:ILE:CB   | 10:C32:670:GLU:H     | 2.27                     | 0.48              |
| 1:R:1445:GLU:HG3    | 2:M:168:LEU:HD12     | 1.96                     | 0.48              |
| 1:R8:1265:PHE:CD2   | 5:P8:684:ARG:CZ      | 2.96                     | 0.48              |
| 2:M8:417:ARG:HH12   | 8:L8:398:ALA:CB      | 2.26                     | 0.48              |
| 2:M8:584:VAL:HG12   | 2:M8:584:VAL:O       | 2.13                     | 0.48              |
| 3:N16:26:ILE:HD12   | 3:N16:40:VAL:CG2     | 2.43                     | 0.48              |
| 5:P:201:ILE:HG13    | 5:P:211:TYR:CE1      | 2.48                     | 0.48              |
| 6:O:23:ARG:CZ       | 6:O:37:GLU:OE1       | 2.61                     | 0.48              |
| 5:P8:655:LEU:HD23   | 5:P8:663:LEU:CD1     | 2.44                     | 0.48              |
| 5:P16:313:TRP:CZ2   | 5:P16:317:ILE:HD11   | 2.48                     | 0.48              |
| 6:O16:60:VAL:HG22   | 6:O16:76:VAL:O       | 2.14                     | 0.48              |
| 8:L8:1069:LEU:CD1   | 9:K8:1086:VAL:HG11   | 2.36                     | 0.48              |
| 10:C16:1477:GLN:HG2 | 24:D8:1407:PHE:CD1   | 2.49                     | 0.48              |
| 10:C16:1549:VAL:O   | 10:C16:1553:VAL:HG23 | 2.13                     | 0.48              |
| 10:C16:1659:ASP:O   | 10:C16:1661:LEU:N    | 2.46                     | 0.48              |
| 10:C16:1814:LYS:HZ3 | 23:J32:738:MET:CG    | 2.26                     | 0.48              |
| 10:C24:705:TYR:O    | 10:C24:794:LYS:NZ    | 2.44                     | 0.48              |
| 10:C24:827:VAL:HG12 | 10:C24:870:ASP:HB3   | 1.96                     | 0.48              |
| 10:C24:1258:LEU:CA  | 10:C24:1323:LEU:CD1  | 2.90                     | 0.48              |
| 11:A40:36:ASN:OD1   | 11:A40:39:GLN:HG3    | 2.13                     | 0.48              |
| 11:A40:558:SER:C    | 11:A40:560:MET:N     | 2.70                     | 0.48              |
| 11:A40:809:VAL:N    | 11:A40:810:PRO:CD    | 2.77                     | 0.48              |
| 12:A:455:LEU:HD23   | 12:A:458:ILE:HD12    | 1.95                     | 0.48              |
| 14:W:739:ARG:NH2    | 15:J:664:GLN:CD      | 2.72                     | 0.48              |
| 10:C:89:LEU:HD11    | 10:C:123:TRP:HE1     | 1.79                     | 0.48              |
| 10:C:667:ILE:CB     | 10:C:670:GLU:H       | 2.27                     | 0.48              |
| 10:C:898:GLN:HE21   | 10:C:1138:GLU:CD     | 2.19                     | 0.48              |
| 10:C:1250:ALA:CB    | 10:C:1309:ARG:HH11   | 2.23                     | 0.48              |
| 10:C:1708:ARG:HH21  | 10:C:1733:ARG:NH2    | 2.10                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:1812:GLU:HA     | 10:C:1819:LEU:HD12   | 1.96                     | 0.48              |
| 10:C8:182:ASP:CB     | 10:C8:183:PRO:HD2    | 2.31                     | 0.48              |
| 10:C8:1282:CYS:HA    | 10:C8:1738:MET:CE    | 2.41                     | 0.48              |
| 10:C8:1549:VAL:O     | 10:C8:1553:VAL:HG23  | 2.13                     | 0.48              |
| 10:C8:1767:LEU:CD1   | 10:C8:1832:MET:HE3   | 2.44                     | 0.48              |
| 11:A16:703:ALA:HA    | 24:D16:1398:ARG:HD2  | 1.90                     | 0.48              |
| 11:A32:72:ILE:HD11   | 21:H24:348:ALA:HA    | 1.94                     | 0.48              |
| 17:F16:72:SER:C      | 17:F16:74:ILE:N      | 2.69                     | 0.48              |
| 18:B:268:GLN:HE22    | 18:B:323:GLU:HG2     | 1.79                     | 0.48              |
| 18:B:968:PHE:CG      | 18:B:1040:MET:CE     | 2.96                     | 0.48              |
| 18:B8:932:THR:HA     | 18:B8:998:LEU:HD12   | 1.95                     | 0.48              |
| 18:B8:990:PRO:C      | 18:B8:992:TRP:N      | 2.71                     | 0.48              |
| 19:4:163:ALA:HB2     | 19:4:218:LEU:CD1     | 2.44                     | 0.48              |
| 20:E:480:MET:CE      | 20:E:493:TRP:CE3     | 2.95                     | 0.48              |
| 22:I:300:LEU:HD11    | 23:J32:689:LEU:HD21  | 1.91                     | 0.48              |
| 21:H8:154:VAL:CG1    | 21:H8:188:ARG:HE     | 2.27                     | 0.48              |
| 21:H16:149:HIS:CD2   | 23:J16:565:ALA:HB3   | 2.48                     | 0.48              |
| 24:D8:1330:ARG:HE    | 24:D8:1332:GLU:HB2   | 1.78                     | 0.48              |
| 10:C32:37:PHE:N      | 10:C32:38:PRO:HD2    | 2.28                     | 0.48              |
| 10:C32:754:MET:CE    | 10:C32:819:GLN:HB3   | 2.42                     | 0.48              |
| 12:A48:305:LEU:HD12  | 12:A48:317:ALA:HB2   | 1.96                     | 0.48              |
| 12:A48:558:SER:C     | 12:A48:560:MET:N     | 2.70                     | 0.48              |
| 2:M:632:VAL:CG2      | 3:N:222:LEU:O        | 2.61                     | 0.48              |
| 2:M8:328:THR:HG21    | 2:M8:350:SER:HB2     | 1.94                     | 0.48              |
| 1:R16:1442:THR:HG21  | 3:N16:13:ILE:HD11    | 1.77                     | 0.48              |
| 4:T:228:ALA:HB2      | 4:T:263:LYS:HE2      | 1.95                     | 0.48              |
| 6:O:288:TRP:CZ3      | 6:O:315:TRP:HH2      | 2.31                     | 0.48              |
| 6:O8:173:VAL:HG22    | 6:O8:189:LEU:HD12    | 1.92                     | 0.48              |
| 6:O8:175:TRP:HZ3     | 6:O8:185:PRO:HB2     | 1.78                     | 0.48              |
| 5:P16:499:TYR:CE1    | 5:P16:527:LYS:HD3    | 2.49                     | 0.48              |
| 5:P16:578:LEU:CD1    | 5:P16:608:LYS:NZ     | 2.76                     | 0.48              |
| 5:P16:655:LEU:HD23   | 5:P16:663:LEU:CD1    | 2.44                     | 0.48              |
| 6:O16:111:LEU:HD11   | 6:O16:129:SER:HA     | 1.96                     | 0.48              |
| 9:K:1150:GLU:OE1     | 9:K:1212:ARG:NH2     | 2.47                     | 0.48              |
| 10:C16:764:ILE:HD13  | 10:C16:781:VAL:HG21  | 1.94                     | 0.48              |
| 10:C16:1767:LEU:CD1  | 10:C16:1832:MET:HE3  | 2.44                     | 0.48              |
| 11:A24:809:VAL:N     | 11:A24:810:PRO:CD    | 2.77                     | 0.48              |
| 10:C24:269:ILE:HG23  | 10:C24:388:TYR:CE1   | 2.49                     | 0.48              |
| 10:C24:1293:THR:HG23 | 10:C24:1369:LEU:HD13 | 1.96                     | 0.48              |
| 13:V:755:LYS:HD2     | 15:J:564:GLN:NE2     | 2.28                     | 0.48              |
| 14:W:473:ARG:HH21    | 14:W:558:LEU:HD12    | 1.79                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:420:TYR:CZ     | 10:C:435:SER:HB3     | 2.48                     | 0.48              |
| 10:C:1285:VAL:HG21  | 10:C:1738:MET:HE2    | 0.50                     | 0.48              |
| 10:C:1659:ASP:O     | 10:C:1661:LEU:N      | 2.46                     | 0.48              |
| 10:C8:553:LEU:HD23  | 10:C8:595:THR:CG2    | 2.44                     | 0.48              |
| 10:C8:1002:LEU:HD23 | 10:C8:1012:ARG:NH1   | 2.26                     | 0.48              |
| 11:A16:676:TYR:CZ   | 24:D16:1395:SER:HB3  | 2.43                     | 0.48              |
| 11:A32:305:LEU:HD12 | 11:A32:317:ALA:HB2   | 1.95                     | 0.48              |
| 18:B:746:LEU:HB2    | 18:B:767:VAL:HG11    | 1.95                     | 0.48              |
| 18:B8:638:ALA:HA    | 18:B8:699:MET:CE     | 2.41                     | 0.48              |
| 18:B8:1031:TRP:CE3  | 18:B8:1041:LEU:HD22  | 2.48                     | 0.48              |
| 18:B8:1098:MET:HE2  | 18:B8:1139:LYS:HA    | 1.95                     | 0.48              |
| 18:B8:1553:SER:OG   | 18:B8:1556:SER:CB    | 2.62                     | 0.48              |
| 19:4:14:GLU:OE2     | 19:4:439:LEU:HD22    | 2.14                     | 0.48              |
| 19:4:103:GLN:CD     | 19:4:411:LEU:CD1     | 2.81                     | 0.48              |
| 20:E:350:GLU:O      | 20:E:352:PHE:N       | 2.47                     | 0.48              |
| 20:E:353:ILE:CG1    | 20:E:413:PHE:CD2     | 2.87                     | 0.48              |
| 20:E:440:VAL:O      | 20:E:442:LYS:N       | 2.46                     | 0.48              |
| 19:48:163:ALA:HB2   | 19:48:218:LEU:CD1    | 2.44                     | 0.48              |
| 20:E8:162:ILE:HG13  | 20:E8:163:ILE:HG13   | 1.96                     | 0.48              |
| 20:E8:174:GLY:HA3   | 20:E8:236:HIS:NE2    | 2.29                     | 0.48              |
| 21:H24:253:ARG:NH1  | 23:J24:614:ASP:OD1   | 2.47                     | 0.48              |
| 21:H16:326:GLY:C    | 21:H16:328:THR:H     | 2.22                     | 0.48              |
| 10:C32:269:ILE:HG23 | 10:C32:388:TYR:CE1   | 2.49                     | 0.48              |
| 10:C32:1133:ILE:CG1 | 10:C32:1152:LYS:HD2  | 2.43                     | 0.48              |
| 10:C32:1767:LEU:CD1 | 10:C32:1832:MET:HE3  | 2.44                     | 0.48              |
| 1:R:1428:VAL:HG23   | 6:O:165:LYS:HZ1      | 1.75                     | 0.48              |
| 3:N:19:MET:CE       | 3:N:23:GLY:HA2       | 2.40                     | 0.48              |
| 3:N8:178:LYS:HE2    | 3:N8:192:LYS:HD2     | 1.95                     | 0.48              |
| 5:P:47:ASN:CG       | 5:P:471:SER:HG       | 2.09                     | 0.48              |
| 5:P:451:LYS:HD2     | 6:O:312:ASN:O        | 2.13                     | 0.48              |
| 5:P8:451:LYS:HD2    | 6:O8:312:ASN:O       | 2.13                     | 0.48              |
| 5:P16:12:GLU:CD     | 5:P16:78:GLY:H       | 2.22                     | 0.48              |
| 5:P16:167:SER:HB3   | 5:P16:398:LYS:HE3    | 1.94                     | 0.48              |
| 5:P16:451:LYS:HD2   | 6:O16:312:ASN:O      | 2.13                     | 0.48              |
| 8:L:1038:MET:CE     | 8:L:1054:HIS:NE2     | 2.77                     | 0.48              |
| 8:L16:1058:ILE:CG2  | 9:K16:1083:ILE:CD1   | 2.92                     | 0.48              |
| 8:L16:1058:ILE:HG23 | 9:K16:1083:ILE:CD1   | 2.44                     | 0.48              |
| 10:C16:667:ILE:HD12 | 10:C16:697:HIS:ND1   | 2.24                     | 0.48              |
| 10:C16:1812:GLU:HA  | 10:C16:1819:LEU:HD12 | 1.95                     | 0.48              |
| 10:C24:1547:LYS:CD  | 24:D24:1406:SER:N    | 2.66                     | 0.48              |
| 10:C24:1733:ARG:NE  | 21:H24:275:LYS:HE2   | 2.19                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A40:88:THR:CG2    | 22:I16:301:LEU:HD21  | 2.43                     | 0.48              |
| 11:A40:257:GLN:CD    | 11:A40:263:ASP:OD1   | 2.51                     | 0.48              |
| 11:A40:362:ARG:CG    | 11:A40:366:ARG:NH2   | 2.75                     | 0.48              |
| 12:A:820:LEU:HD22    | 12:A:830:ILE:HG23    | 1.96                     | 0.48              |
| 15:J:722:LEU:HD22    | 10:C8:1623:ILE:CG1   | 2.37                     | 0.48              |
| 10:C:470:HIS:CD2     | 10:C:508:ILE:HD11    | 2.44                     | 0.48              |
| 10:C:1282:CYS:HA     | 10:C:1738:MET:CE     | 2.41                     | 0.48              |
| 10:C:1599:ASP:CG     | 10:C:1604:VAL:HG23   | 2.39                     | 0.48              |
| 10:C8:667:ILE:CB     | 10:C8:670:GLU:H      | 2.26                     | 0.48              |
| 10:C8:667:ILE:HG22   | 10:C8:670:GLU:H      | 1.78                     | 0.48              |
| 11:A16:362:ARG:CG    | 11:A16:366:ARG:NH2   | 2.75                     | 0.48              |
| 11:A16:820:LEU:HD22  | 11:A16:830:ILE:HG23  | 1.96                     | 0.48              |
| 11:A32:148:LEU:CD1   | 18:B8:1956:ILE:HD13  | 2.40                     | 0.48              |
| 11:A32:558:SER:C     | 11:A32:560:MET:N     | 2.70                     | 0.48              |
| 18:B:1101:TYR:CE1    | 18:B:1105:LEU:CD1    | 2.93                     | 0.48              |
| 18:B8:268:GLN:HE22   | 18:B8:323:GLU:HG2    | 1.79                     | 0.48              |
| 18:B8:1317:THR:O     | 18:B8:1321:MET:HG2   | 2.14                     | 0.48              |
| 19:4:57:ASN:C        | 19:4:59:GLY:N        | 2.72                     | 0.48              |
| 19:4:122:GLN:HG2     | 19:4:140:THR:CG2     | 2.43                     | 0.48              |
| 19:48:57:ASN:C       | 19:48:59:GLY:N       | 2.72                     | 0.48              |
| 23:J32:686:MET:SD    | 23:J32:694:ARG:CZ    | 3.01                     | 0.48              |
| 10:C32:1488:ILE:HG21 | 10:C32:1525:VAL:HG13 | 1.95                     | 0.48              |
| 1:R:1420:PHE:O       | 1:R:1423:SER:OG      | 2.32                     | 0.48              |
| 1:R8:1445:GLU:HG3    | 2:M8:168:LEU:HD12    | 1.96                     | 0.48              |
| 2:M8:173:SER:HG      | 3:N8:234:GLN:HE22    | 1.58                     | 0.48              |
| 1:R16:1266:THR:HG23  | 5:P16:680:ILE:CG2    | 2.32                     | 0.48              |
| 1:R16:1442:THR:CG2   | 3:N16:13:ILE:HD12    | 2.33                     | 0.48              |
| 2:M16:200:THR:HG21   | 3:N16:14:VAL:HB      | 1.95                     | 0.48              |
| 3:N16:222:LEU:CD1    | 3:N16:270:THR:HA     | 2.44                     | 0.48              |
| 5:P:313:TRP:CZ2      | 5:P:317:ILE:HD11     | 2.49                     | 0.48              |
| 5:P8:12:GLU:CD       | 5:P8:78:GLY:H        | 2.22                     | 0.48              |
| 6:O8:180:GLY:O       | 6:O8:182:GLU:N       | 2.47                     | 0.48              |
| 5:P16:233:TYR:CE1    | 5:P16:237:MET:HE2    | 2.48                     | 0.48              |
| 5:P16:568:SER:OG     | 5:P16:581:TRP:NE1    | 2.47                     | 0.48              |
| 7:Q16:10:VAL:HG21    | 7:Q16:327:LEU:CD2    | 2.43                     | 0.48              |
| 8:L:1096:GLU:OE2     | 9:K:996:MET:HB3      | 2.13                     | 0.48              |
| 9:K:738:GLN:OE1      | 9:K:756:ASN:HB2      | 2.13                     | 0.48              |
| 9:K8:1279:GLU:O      | 9:K8:1280:PHE:C      | 2.51                     | 0.48              |
| 10:C16:827:VAL:HG12  | 10:C16:870:ASP:HB3   | 1.96                     | 0.48              |
| 10:C16:1541:PHE:CE1  | 10:C16:1649:LYS:CD   | 2.89                     | 0.48              |
| 10:C24:89:LEU:HD11   | 10:C24:123:TRP:HE1   | 1.79                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C24:667:ILE:HD12 | 10:C24:697:HIS:ND1  | 2.24                     | 0.48              |
| 10:C24:1394:GLN:OE1 | 24:D24:1158:SER:OG  | 2.22                     | 0.48              |
| 10:C24:1767:LEU:CD1 | 10:C24:1832:MET:HE3 | 2.44                     | 0.48              |
| 13:V:790:GLN:HE21   | 14:W:674:GLN:NE2    | 1.94                     | 0.48              |
| 10:C:919:ASP:H      | 10:C:927:THR:HG21   | 1.79                     | 0.48              |
| 10:C:1624:LEU:HD22  | 10:C:1628:SER:HB2   | 1.92                     | 0.48              |
| 10:C8:412:MET:O     | 10:C8:416:VAL:HG23  | 2.13                     | 0.48              |
| 10:C8:664:ASN:O     | 10:C8:668:ALA:N     | 2.42                     | 0.48              |
| 10:C8:1599:ASP:CG   | 10:C8:1604:VAL:HG23 | 2.39                     | 0.48              |
| 11:A16:557:LEU:HD23 | 11:A16:561:ASP:CB   | 2.44                     | 0.48              |
| 11:A16:707:LEU:HD21 | 11:A16:767:ARG:HH22 | 1.59                     | 0.48              |
| 11:A32:711:ARG:HG2  | 11:A32:713:ASP:OD1  | 2.14                     | 0.48              |
| 18:B:789:LEU:HD11   | 18:B:848:PHE:CE1    | 2.49                     | 0.48              |
| 18:B:846:SER:CB     | 18:B:899:LYS:HZ3    | 2.07                     | 0.48              |
| 18:B:1031:TRP:CE3   | 18:B:1041:LEU:HD22  | 2.48                     | 0.48              |
| 18:B:1298:GLN:HG2   | 18:B:1303:ILE:HD12  | 1.96                     | 0.48              |
| 18:B8:1688:ALA:O    | 18:B8:1692:VAL:HG23 | 2.14                     | 0.48              |
| 19:4:345:GLU:HB3    | 19:4:349:LEU:CD1    | 2.44                     | 0.48              |
| 20:E:162:ILE:HG13   | 20:E:163:ILE:HG13   | 1.96                     | 0.48              |
| 20:E:343:THR:HA     | 20:E:344:PRO:HD3    | 1.60                     | 0.48              |
| 21:H:322:LEU:CD2    | 22:I:300:LEU:HD11   | 2.44                     | 0.48              |
| 21:H24:145:TYR:HB3  | 21:H24:148:GLN:HE21 | 1.79                     | 0.48              |
| 21:H24:154:VAL:CG1  | 21:H24:188:ARG:HE   | 2.27                     | 0.48              |
| 23:J16:686:MET:SD   | 23:J16:694:ARG:CZ   | 3.01                     | 0.48              |
| 10:C32:758:GLN:HE21 | 10:C32:819:GLN:CG   | 2.24                     | 0.48              |
| 10:C32:1282:CYS:HA  | 10:C32:1738:MET:CE  | 2.41                     | 0.48              |
| 1:R:1175:TYR:CA     | 1:R:1177:TRP:CZ3    | 2.79                     | 0.47              |
| 1:R:1324:ASP:OD2    | 10:C:1180:ILE:HB    | 2.13                     | 0.47              |
| 1:R:1340:LEU:HD13   | 1:R:1354:VAL:HG21   | 1.96                     | 0.47              |
| 1:R:1472:HIS:CE1    | 1:R:1476:LEU:HD11   | 2.49                     | 0.47              |
| 2:M:246:ALA:C       | 2:M:290:ILE:CD1     | 2.86                     | 0.47              |
| 2:M:562:PHE:CE2     | 3:N:295:GLU:OE2     | 2.67                     | 0.47              |
| 2:M:772:PHE:CE1     | 2:M:776:LEU:HD12    | 2.49                     | 0.47              |
| 1:R8:983:ARG:CZ     | 24:D40:1364:PRO:O   | 2.62                     | 0.47              |
| 2:M16:411:ILE:CG2   | 8:L16:397:CYS:SG    | 3.02                     | 0.47              |
| 5:P:85:ASP:HB2      | 5:P:86:PRO:HD3      | 1.96                     | 0.47              |
| 5:P:280:LEU:HB3     | 5:P:345:MET:HE1     | 1.95                     | 0.47              |
| 6:O:60:VAL:HG22     | 6:O:76:VAL:O        | 2.14                     | 0.47              |
| 6:O:282:GLU:CB      | 6:O:284:TRP:CZ2     | 2.93                     | 0.47              |
| 5:P8:57:PRO:CG      | 6:O8:29:LEU:HD11    | 2.44                     | 0.47              |
| 5:P16:57:PRO:CG     | 6:O16:29:LEU:HD11   | 2.44                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:O16:54:VAL:CG1     | 6:O16:85:TRP:HE1     | 2.15                     | 0.47              |
| 6:O16:282:GLU:HB2    | 6:O16:284:TRP:CE2    | 2.48                     | 0.47              |
| 10:C16:1061:ASN:O    | 10:C16:1063:PRO:CD   | 2.62                     | 0.47              |
| 10:C16:1599:ASP:CG   | 10:C16:1604:VAL:HG23 | 2.39                     | 0.47              |
| 11:A24:156:MET:CA    | 11:A24:555:HIS:NE2   | 2.77                     | 0.47              |
| 11:A24:362:ARG:CG    | 11:A24:366:ARG:NH2   | 2.75                     | 0.47              |
| 11:A24:455:LEU:HD23  | 11:A24:458:ILE:HD12  | 1.95                     | 0.47              |
| 10:C24:798:VAL:HG12  | 10:C24:802:TRP:CD2   | 2.48                     | 0.47              |
| 11:A40:803:PRO:CA    | 24:D24:1401:LEU:CD1  | 2.91                     | 0.47              |
| 12:A:557:LEU:HD23    | 12:A:561:ASP:CB      | 2.44                     | 0.47              |
| 10:C:381:ILE:CG2     | 10:C:385:TYR:CZ      | 2.97                     | 0.47              |
| 10:C:979:MET:HE1     | 10:C:1028:ILE:CB     | 2.45                     | 0.47              |
| 10:C8:269:ILE:HG23   | 10:C8:388:TYR:CE1    | 2.49                     | 0.47              |
| 10:C8:619:LEU:CB     | 10:C8:620:PRO:CD     | 2.79                     | 0.47              |
| 10:C8:1061:ASN:O     | 10:C8:1063:PRO:CD    | 2.62                     | 0.47              |
| 11:A16:388:VAL:CG2   | 11:A16:459:ARG:HH22  | 2.26                     | 0.47              |
| 11:A16:558:SER:C     | 11:A16:560:MET:N     | 2.70                     | 0.47              |
| 11:A16:702:GLU:OE1   | 24:D16:1393:GLY:O    | 2.31                     | 0.47              |
| 11:A16:711:ARG:CD    | 24:D16:1398:ARG:CG   | 2.88                     | 0.47              |
| 18:B:503:SER:H       | 18:B:504:PRO:HD3     | 1.79                     | 0.47              |
| 18:B:932:THR:HA      | 18:B:998:LEU:HD12    | 1.95                     | 0.47              |
| 18:B8:503:SER:H      | 18:B8:504:PRO:HD3    | 1.79                     | 0.47              |
| 18:B8:1618:HIS:ND1   | 18:B8:1622:ILE:CD1   | 2.74                     | 0.47              |
| 20:E:197:LEU:HD21    | 20:E:201:LEU:HD13    | 1.96                     | 0.47              |
| 19:48:295:SER:OG     | 24:D8:179:PRO:HG2    | 2.13                     | 0.47              |
| 20:E8:350:GLU:O      | 20:E8:352:PHE:N      | 2.47                     | 0.47              |
| 21:H:215:ARG:NH1     | 21:H:219:LYS:NZ      | 2.61                     | 0.47              |
| 22:I8:131:ARG:CG     | 23:J8:557:ARG:CZ     | 2.64                     | 0.47              |
| 22:I8:300:LEU:CG     | 23:J8:689:LEU:HD21   | 2.41                     | 0.47              |
| 21:H24:149:HIS:CD2   | 23:J24:565:ALA:HB3   | 2.48                     | 0.47              |
| 21:H24:215:ARG:NH1   | 21:H24:219:LYS:NZ    | 2.61                     | 0.47              |
| 21:H16:154:VAL:CG1   | 21:H16:188:ARG:HE    | 2.27                     | 0.47              |
| 24:D:1099:ARG:NH1    | 24:D:1149:VAL:HG11   | 2.28                     | 0.47              |
| 10:C32:460:TRP:CD1   | 10:C32:495:LYS:HZ3   | 2.32                     | 0.47              |
| 10:C32:988:GLN:HE21  | 10:C32:1064:PHE:HE1  | 1.59                     | 0.47              |
| 10:C32:1624:LEU:HD22 | 10:C32:1628:SER:HB2  | 1.92                     | 0.47              |
| 10:C32:1812:GLU:HA   | 10:C32:1819:LEU:HD12 | 1.96                     | 0.47              |
| 12:A48:388:VAL:CB    | 12:A48:459:ARG:HH12  | 2.26                     | 0.47              |
| 12:A48:455:LEU:HD23  | 12:A48:458:ILE:HD12  | 1.95                     | 0.47              |
| 12:A48:711:ARG:HG2   | 12:A48:713:ASP:OD1   | 2.14                     | 0.47              |
| 1:R8:1190:VAL:HG22   | 24:D40:1456:GLU:CB   | 2.44                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R8:1239:TRP:CD2    | 1:R8:1251:LEU:HD13   | 2.49                     | 0.47              |
| 2:M8:562:PHE:CE2     | 3:N8:295:GLU:OE2     | 2.67                     | 0.47              |
| 2:M8:772:PHE:CZ      | 2:M8:776:LEU:HD11    | 2.49                     | 0.47              |
| 3:N8:2:PRO:C         | 3:N8:3:GLY:O         | 2.56                     | 0.47              |
| 1:R16:1239:TRP:CD2   | 1:R16:1251:LEU:HD13  | 2.49                     | 0.47              |
| 1:R16:1340:LEU:HD13  | 1:R16:1354:VAL:HG21  | 1.96                     | 0.47              |
| 1:R16:1379:GLN:O     | 1:R16:1380:LYS:C     | 2.56                     | 0.47              |
| 2:M16:772:PHE:CZ     | 2:M16:776:LEU:HD11   | 2.50                     | 0.47              |
| 6:O:180:GLY:O        | 6:O:182:GLU:N        | 2.47                     | 0.47              |
| 8:L8:1038:MET:CE     | 8:L8:1054:HIS:NE2    | 2.77                     | 0.47              |
| 9:K:847:LEU:HD22     | 9:K:910:SER:CB       | 2.43                     | 0.47              |
| 9:K:1110:GLN:NE2     | 9:K:1127:PHE:H       | 2.11                     | 0.47              |
| 9:K8:1150:GLU:OE1    | 9:K8:1212:ARG:NH2    | 2.47                     | 0.47              |
| 10:C16:37:PHE:N      | 10:C16:38:PRO:HD2    | 2.28                     | 0.47              |
| 10:C16:1220:SER:HA   | 10:C16:1225:ARG:NH2  | 2.28                     | 0.47              |
| 10:C16:1293:THR:HG23 | 10:C16:1369:LEU:HD13 | 1.96                     | 0.47              |
| 11:A24:388:VAL:CB    | 11:A24:459:ARG:HH12  | 2.26                     | 0.47              |
| 11:A40:305:LEU:HD12  | 11:A40:317:ALA:HB2   | 1.96                     | 0.47              |
| 11:A40:388:VAL:CB    | 11:A40:459:ARG:HH12  | 2.26                     | 0.47              |
| 11:A40:557:LEU:HD23  | 11:A40:561:ASP:CB    | 2.44                     | 0.47              |
| 10:C:37:PHE:N        | 10:C:38:PRO:HD2      | 2.28                     | 0.47              |
| 10:C8:1033:GLY:C     | 10:C8:1218:ARG:NH2   | 2.70                     | 0.47              |
| 11:A16:72:ILE:HD11   | 21:H:348:ALA:HA      | 1.94                     | 0.47              |
| 18:B:475:GLU:O       | 18:B:479:PRO:HG2     | 2.14                     | 0.47              |
| 18:B:1059:SER:O      | 18:B:1062:SER:OG     | 2.25                     | 0.47              |
| 18:B:1317:THR:O      | 18:B:1321:MET:HG2    | 2.14                     | 0.47              |
| 18:B:1553:SER:OG     | 18:B:1556:SER:CB     | 2.62                     | 0.47              |
| 18:B:1688:ALA:O      | 18:B:1692:VAL:HG23   | 2.14                     | 0.47              |
| 18:B8:113:TYR:C      | 18:B8:114:GLY:O      | 2.57                     | 0.47              |
| 18:B8:1342:LEU:CD2   | 18:B8:1406:ALA:HB3   | 2.42                     | 0.47              |
| 19:4:56:GLU:C        | 19:4:58:GLU:H        | 2.21                     | 0.47              |
| 19:48:345:GLU:HB3    | 19:48:349:LEU:CD1    | 2.44                     | 0.47              |
| 20:E8:31:PHE:HE1     | 20:E8:46:PHE:HZ      | 1.62                     | 0.47              |
| 20:E8:432:ILE:CG2    | 24:D40:72:GLU:OE1    | 2.57                     | 0.47              |
| 24:D40:749:ARG:HH12  | 24:D40:964:LEU:C     | 2.22                     | 0.47              |
| 10:C32:381:ILE:CG2   | 10:C32:385:TYR:CZ    | 2.97                     | 0.47              |
| 10:C32:919:ASP:H     | 10:C32:927:THR:HG21  | 1.79                     | 0.47              |
| 12:A48:798:PHE:HZ    | 12:A48:847:ARG:NH1   | 2.01                     | 0.47              |
| 1:R:1194:ARG:O       | 1:R:1195:ARG:C       | 2.52                     | 0.47              |
| 1:R8:983:ARG:O       | 24:D40:1360:ALA:HB3  | 1.97                     | 0.47              |
| 1:R8:1420:PHE:O      | 1:R8:1423:SER:OG     | 2.32                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:540:TYR:HD1     | 2:M8:555:LEU:HD22    | 1.75                     | 0.47              |
| 2:M8:651:ARG:HG3     | 2:M8:664:MET:CE      | 2.42                     | 0.47              |
| 5:P:568:SER:OG       | 5:P:581:TRP:NE1      | 2.47                     | 0.47              |
| 5:P8:568:SER:OG      | 5:P8:581:TRP:NE1     | 2.47                     | 0.47              |
| 9:K:1019:ARG:CZ      | 9:K:1059:ARG:CG      | 2.92                     | 0.47              |
| 10:C16:89:LEU:HD11   | 10:C16:123:TRP:HE1   | 1.79                     | 0.47              |
| 10:C16:754:MET:CE    | 10:C16:819:GLN:HB3   | 2.42                     | 0.47              |
| 10:C16:1133:ILE:CG1  | 10:C16:1152:LYS:HD2  | 2.43                     | 0.47              |
| 10:C16:1530:PHE:CE1  | 11:A24:132:MET:CE    | 2.92                     | 0.47              |
| 10:C16:1616:ILE:C    | 10:C16:1618:SER:N    | 2.70                     | 0.47              |
| 10:C16:1708:ARG:NH1  | 21:H:279:GLU:CB      | 2.63                     | 0.47              |
| 10:C24:1061:ASN:O    | 10:C24:1063:PRO:CD   | 2.62                     | 0.47              |
| 10:C24:1078:GLY:O    | 10:C24:1080:SER:N    | 2.46                     | 0.47              |
| 10:C24:1610:MET:HG2  | 10:C24:1614:LEU:HD12 | 1.96                     | 0.47              |
| 11:A40:390:ALA:HB3   | 24:D32:1099:ARG:HB2  | 1.86                     | 0.47              |
| 12:A:711:ARG:HG2     | 12:A:713:ASP:OD1     | 2.14                     | 0.47              |
| 14:W:697:ARG:O       | 14:W:700:SER:OG      | 2.27                     | 0.47              |
| 10:C:1624:LEU:HD23   | 10:C:1628:SER:CB     | 2.38                     | 0.47              |
| 10:C8:919:ASP:H      | 10:C8:927:THR:HG21   | 1.79                     | 0.47              |
| 10:C8:1424:GLN:HE22  | 10:C8:1478:VAL:CG1   | 2.27                     | 0.47              |
| 11:A32:72:ILE:HD13   | 21:H24:348:ALA:HA    | 1.95                     | 0.47              |
| 11:A32:445:ASN:ND2   | 17:F24:65:ARG:NH1    | 2.59                     | 0.47              |
| 18:B:712:PRO:HG3     | 18:B:759:MET:HE2     | 1.84                     | 0.47              |
| 18:B8:287:MET:HE3    | 18:B8:297:GLY:HA3    | 1.96                     | 0.47              |
| 18:B8:968:PHE:CG     | 18:B8:1040:MET:CE    | 2.96                     | 0.47              |
| 20:E8:343:THR:CB     | 20:E8:344:PRO:HD2    | 2.44                     | 0.47              |
| 21:H:136:TYR:CE2     | 23:J32:554:LEU:HD13  | 2.49                     | 0.47              |
| 21:H:326:GLY:C       | 21:H:328:THR:H       | 2.22                     | 0.47              |
| 22:I:333:ARG:NH2     | 22:I:350:PHE:HB2     | 2.30                     | 0.47              |
| 21:H8:136:TYR:CE2    | 23:J8:554:LEU:HD13   | 2.49                     | 0.47              |
| 21:H8:154:VAL:HG21   | 21:H8:188:ARG:NH2    | 2.30                     | 0.47              |
| 21:H16:154:VAL:HG21  | 21:H16:188:ARG:NH2   | 2.30                     | 0.47              |
| 10:C32:1424:GLN:HE21 | 10:C32:1478:VAL:HG13 | 1.71                     | 0.47              |
| 10:C32:1659:ASP:O    | 10:C32:1661:LEU:N    | 2.46                     | 0.47              |
| 2:M:627:TYR:HD1      | 2:M:631:THR:HG1      | 1.61                     | 0.47              |
| 2:M:739:TYR:CE1      | 2:M:798:MET:CE       | 2.97                     | 0.47              |
| 2:M16:584:VAL:HG12   | 2:M16:584:VAL:O      | 2.13                     | 0.47              |
| 7:Q:219:GLY:C        | 7:Q:221:TRP:N        | 2.73                     | 0.47              |
| 7:Q:235:ILE:HD13     | 7:Q:243:CYS:CB       | 2.45                     | 0.47              |
| 5:P16:16:PHE:HD1     | 6:O16:311:LEU:HD12   | 1.75                     | 0.47              |
| 7:Q16:235:ILE:HD13   | 7:Q16:243:CYS:CB     | 2.45                     | 0.47              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 9:K:743:ARG:NH2     | 9:K:772:TYR:CE1      | 2.82                     | 0.47              |
| 10:C16:758:GLN:HE21 | 10:C16:819:GLN:CG    | 2.24                     | 0.47              |
| 10:C16:847:ARG:HH22 | 10:C16:912:THR:H     | 1.62                     | 0.47              |
| 10:C16:1283:LEU:CD1 | 10:C16:1357:LEU:HD11 | 2.40                     | 0.47              |
| 11:A24:440:LEU:HB2  | 11:A24:443:LEU:HD11  | 1.75                     | 0.47              |
| 10:C24:460:TRP:CD1  | 10:C24:495:LYS:HZ3   | 2.32                     | 0.47              |
| 10:C24:768:ARG:HH22 | 10:C24:775:LYS:HG2   | 1.67                     | 0.47              |
| 10:C24:1278:ASP:OD2 | 21:H24:283:LYS:CA    | 2.60                     | 0.47              |
| 13:V:798:LEU:HD12   | 15:J:606:ILE:HG12    | 1.96                     | 0.47              |
| 13:V:818:THR:HG23   | 13:V:824:TRP:CZ2     | 2.50                     | 0.47              |
| 10:C:453:LEU:HD22   | 10:C:459:LEU:HD21    | 0.51                     | 0.47              |
| 10:C:1154:TRP:NE1   | 10:C:1158:HIS:CE1    | 2.82                     | 0.47              |
| 10:C:1610:MET:HG2   | 10:C:1614:LEU:HD12   | 1.97                     | 0.47              |
| 10:C8:89:LEU:HD11   | 10:C8:123:TRP:HE1    | 1.79                     | 0.47              |
| 10:C8:381:ILE:CG2   | 10:C8:385:TYR:CZ     | 2.97                     | 0.47              |
| 10:C8:619:LEU:CB    | 10:C8:620:PRO:HD2    | 2.23                     | 0.47              |
| 10:C8:1812:GLU:HA   | 10:C8:1819:LEU:HD12  | 1.96                     | 0.47              |
| 11:A32:820:LEU:HD22 | 11:A32:830:ILE:HG23  | 1.96                     | 0.47              |
| 18:B:7:VAL:HG12     | 18:B:11:LEU:HD12     | 1.97                     | 0.47              |
| 18:B:1110:LEU:HD13  | 21:H:323:TYR:CE1     | 2.47                     | 0.47              |
| 18:B:1110:LEU:HD21  | 21:H:326:GLY:HA2     | 1.77                     | 0.47              |
| 18:B8:729:LEU:CD1   | 18:B8:1196:MET:SD    | 3.03                     | 0.47              |
| 18:B8:1161:LEU:CD2  | 18:B8:1403:ILE:HD12  | 2.41                     | 0.47              |
| 19:4:286:TRP:NE1    | 20:E:163:ILE:HG23    | 2.28                     | 0.47              |
| 19:48:56:GLU:C      | 19:48:58:GLU:H       | 2.21                     | 0.47              |
| 19:48:286:TRP:NE1   | 20:E8:163:ILE:HG23   | 2.28                     | 0.47              |
| 19:48:337:HIS:CE1   | 24:D8:139:GLU:CD     | 2.93                     | 0.47              |
| 20:E8:197:LEU:HD21  | 20:E8:201:LEU:HD13   | 1.96                     | 0.47              |
| 23:J32:686:MET:CE   | 23:J32:694:ARG:NE    | 2.67                     | 0.47              |
| 21:H8:326:GLY:C     | 21:H8:328:THR:H      | 2.22                     | 0.47              |
| 22:I24:203:GLN:N    | 22:I24:204:PRO:HD2   | 2.29                     | 0.47              |
| 22:I24:333:ARG:NH2  | 22:I24:350:PHE:HB2   | 2.30                     | 0.47              |
| 23:J24:686:MET:SD   | 23:J24:694:ARG:CZ    | 3.01                     | 0.47              |
| 24:D24:274:MET:CE   | 24:D24:321:SER:HB2   | 2.40                     | 0.47              |
| 1:R:768:LEU:HD11    | 24:D:1362:VAL:O      | 2.07                     | 0.47              |
| 1:R:1239:TRP:CD2    | 1:R:1251:LEU:HD13    | 2.49                     | 0.47              |
| 3:N:208:LYS:HB2     | 3:N:241:TRP:HH2      | 1.80                     | 0.47              |
| 1:R8:1449:TRP:CZ3   | 2:M8:160:LEU:HD11    | 2.36                     | 0.47              |
| 2:M8:415:ASP:OD2    | 2:M8:456:ARG:NH2     | 2.43                     | 0.47              |
| 2:M16:562:PHE:CE2   | 3:N16:295:GLU:OE2    | 2.67                     | 0.47              |
| 5:P:251:LYS:CE      | 14:W:765:LYS:CE      | 2.83                     | 0.47              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 6:O:173:VAL:CG2     | 6:O:189:LEU:CD1      | 2.85                     | 0.47              |
| 5:P16:280:LEU:HB3   | 5:P16:345:MET:HE1    | 1.95                     | 0.47              |
| 8:L16:1026:ARG:CD   | 9:K16:1284:MET:CB    | 2.84                     | 0.47              |
| 9:K:714:ARG:NH2     | 9:K:729:VAL:O        | 2.48                     | 0.47              |
| 9:K8:1160:ARG:HH22  | 9:K8:1220:ASN:ND2    | 2.10                     | 0.47              |
| 10:C16:381:ILE:CG2  | 10:C16:385:TYR:CZ    | 2.97                     | 0.47              |
| 10:C16:453:LEU:HD22 | 10:C16:459:LEU:HD21  | 0.51                     | 0.47              |
| 10:C16:1591:LYS:NZ  | 11:A24:139:ASP:OD2   | 2.34                     | 0.47              |
| 11:A24:305:LEU:HD12 | 11:A24:317:ALA:HB2   | 1.96                     | 0.47              |
| 11:A24:557:LEU:HD23 | 11:A24:561:ASP:CB    | 2.44                     | 0.47              |
| 10:C24:300:VAL:CG1  | 10:C24:317:ARG:CG    | 2.88                     | 0.47              |
| 10:C24:1599:ASP:CG  | 10:C24:1604:VAL:HG23 | 2.39                     | 0.47              |
| 12:A:557:LEU:CD2    | 12:A:561:ASP:CB      | 2.90                     | 0.47              |
| 14:W:370:VAL:HG21   | 14:W:474:ILE:HD13    | 1.97                     | 0.47              |
| 10:C:553:LEU:HD23   | 10:C:595:THR:CG2     | 2.44                     | 0.47              |
| 10:C:988:GLN:HE21   | 10:C:1064:PHE:HE1    | 1.59                     | 0.47              |
| 10:C8:827:VAL:HG12  | 10:C8:870:ASP:HB3    | 1.96                     | 0.47              |
| 10:C8:1488:ILE:CG2  | 10:C8:1525:VAL:HG13  | 2.45                     | 0.47              |
| 18:B8:366:ALA:HB1   | 18:B8:369:SER:OG     | 2.15                     | 0.47              |
| 18:B8:628:VAL:HA    | 18:B8:631:LEU:HD12   | 1.95                     | 0.47              |
| 18:B8:789:LEU:HD11  | 18:B8:848:PHE:CE1    | 2.49                     | 0.47              |
| 18:B8:1660:SER:HA   | 18:B8:1724:MET:HE1   | 1.96                     | 0.47              |
| 19:48:444:HIS:C     | 19:48:446:LEU:H      | 2.23                     | 0.47              |
| 22:I:178:LEU:HD12   | 23:J32:599:LEU:HD22  | 1.95                     | 0.47              |
| 21:H8:145:TYR:HB3   | 21:H8:148:GLN:HE21   | 1.79                     | 0.47              |
| 21:H8:322:LEU:CD2   | 22:I8:300:LEU:HD11   | 2.44                     | 0.47              |
| 21:H24:154:VAL:HG21 | 21:H24:188:ARG:NH2   | 2.30                     | 0.47              |
| 23:J16:686:MET:CE   | 23:J16:694:ARG:NE    | 2.67                     | 0.47              |
| 24:D8:853:MET:CB    | 24:D8:885:TYR:CE2    | 2.84                     | 0.47              |
| 10:C32:572:ILE:C    | 10:C32:574:PRO:HD2   | 2.40                     | 0.47              |
| 10:C32:798:VAL:HG12 | 10:C32:802:TRP:CD2   | 2.48                     | 0.47              |
| 10:C32:827:VAL:HG12 | 10:C32:870:ASP:HB3   | 1.96                     | 0.47              |
| 10:C32:1488:ILE:CG2 | 10:C32:1525:VAL:HG13 | 2.45                     | 0.47              |
| 1:R:1079:ASP:OD1    | 5:P:713:LEU:HB3      | 2.14                     | 0.47              |
| 1:R:1428:VAL:HG13   | 1:R:1431:ARG:HE      | 1.79                     | 0.47              |
| 2:M8:544:LEU:HD21   | 2:M8:586:ALA:HB3     | 1.91                     | 0.47              |
| 3:N8:26:ILE:HD12    | 3:N8:40:VAL:CG2      | 2.44                     | 0.47              |
| 3:N8:260:THR:OG1    | 3:N8:261:PRO:HD2     | 2.15                     | 0.47              |
| 3:N16:202:CYS:O     | 3:N16:204:PRO:O      | 2.33                     | 0.47              |
| 5:P:57:PRO:CG       | 6:O:29:LEU:HD11      | 2.44                     | 0.47              |
| 6:O:282:GLU:HB2     | 6:O:284:TRP:CE2      | 2.49                     | 0.47              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P8:201:ILE:HG13    | 5:P8:211:TYR:CE1    | 2.48                     | 0.47              |
| 5:P8:614:VAL:HG21    | 5:P8:629:ARG:NE     | 2.29                     | 0.47              |
| 6:O16:133:LEU:HD11   | 6:O16:153:PHE:CE1   | 2.47                     | 0.47              |
| 9:K:879:CYS:HB3      | 9:K:900:TYR:CE2     | 2.50                     | 0.47              |
| 9:K8:716:ALA:HB1     | 10:C32:503:THR:CG2  | 2.43                     | 0.47              |
| 10:C16:764:ILE:CD1   | 10:C16:781:VAL:CG2  | 2.86                     | 0.47              |
| 10:C16:1453:ARG:HH12 | 24:D8:1150:GLY:HA3  | 1.79                     | 0.47              |
| 10:C24:1477:GLN:CG   | 24:D24:1407:PHE:CD1 | 2.98                     | 0.47              |
| 11:A40:156:MET:HE1   | 11:A40:555:HIS:C    | 2.39                     | 0.47              |
| 11:A40:711:ARG:HG2   | 11:A40:713:ASP:OD1  | 2.14                     | 0.47              |
| 11:A40:743:ARG:HH22  | 24:D32:699:HIS:CE1  | 2.30                     | 0.47              |
| 12:A:643:SER:HA      | 12:A:682:LEU:CD2    | 2.45                     | 0.47              |
| 13:V:850:LEU:HD21    | 15:J:662:THR:HA     | 1.97                     | 0.47              |
| 14:W:638:VAL:CG2     | 15:J:561:PHE:CZ     | 2.97                     | 0.47              |
| 10:C:281:ASP:OD2     | 24:D:1398:ARG:CG    | 2.63                     | 0.47              |
| 10:C:386:ASN:O       | 10:C:390:HIS:HD2    | 1.89                     | 0.47              |
| 10:C:572:ILE:C       | 10:C:574:PRO:HD2    | 2.40                     | 0.47              |
| 10:C:827:VAL:HG12    | 10:C:870:ASP:HB3    | 1.96                     | 0.47              |
| 10:C:1488:ILE:HG21   | 10:C:1525:VAL:HG13  | 1.96                     | 0.47              |
| 10:C:1708:ARG:HH21   | 10:C:1733:ARG:CZ    | 2.27                     | 0.47              |
| 11:A32:711:ARG:CD    | 24:D32:1398:ARG:CG  | 2.91                     | 0.47              |
| 11:A32:809:VAL:N     | 11:A32:810:PRO:CD   | 2.77                     | 0.47              |
| 18:B:1424:LEU:HD23   | 18:B:1490:ILE:CD1   | 2.45                     | 0.47              |
| 18:B8:1806:HIS:C     | 18:B8:1808:GLY:H    | 2.22                     | 0.47              |
| 18:B8:1911:LEU:CB    | 18:B8:1960:LEU:HD12 | 2.45                     | 0.47              |
| 19:4:346:ILE:CG2     | 19:4:347:ALA:N      | 2.77                     | 0.47              |
| 20:E:174:GLY:HA3     | 20:E:236:HIS:NE2    | 2.29                     | 0.47              |
| 20:E:447:ILE:HG22    | 20:E:451:ILE:HB     | 1.97                     | 0.47              |
| 20:E8:473:LEU:CD2    | 20:E8:480:MET:SD    | 3.01                     | 0.47              |
| 21:H:145:TYR:HB3     | 21:H:148:GLN:HE21   | 1.79                     | 0.47              |
| 21:H:154:VAL:CG1     | 21:H:188:ARG:HE     | 2.27                     | 0.47              |
| 21:H:154:VAL:HG21    | 21:H:188:ARG:NH2    | 2.30                     | 0.47              |
| 21:H:322:LEU:CG      | 22:I:300:LEU:HD11   | 2.39                     | 0.47              |
| 23:J8:686:MET:CE     | 23:J8:694:ARG:NE    | 2.67                     | 0.47              |
| 21:H16:136:TYR:CE2   | 23:J16:554:LEU:HD13 | 2.49                     | 0.47              |
| 21:H16:321:SER:O     | 21:H16:323:TYR:CD1  | 2.68                     | 0.47              |
| 12:A48:259:ILE:HG23  | 12:A48:276:LEU:HD22 | 1.96                     | 0.47              |
| 12:A48:557:LEU:HD23  | 12:A48:561:ASP:CB   | 2.44                     | 0.47              |
| 1:R:1360:GLN:O       | 10:C:608:ASP:OD2    | 2.32                     | 0.47              |
| 2:M:200:THR:HG21     | 3:N:14:VAL:HB       | 1.95                     | 0.47              |
| 2:M:415:ASP:OD2      | 2:M:456:ARG:NH2     | 2.43                     | 0.47              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 2:M:625:HIS:HE2      | 3:N:225:PRO:CA      | 2.26                     | 0.47              |
| 2:M:772:PHE:CZ       | 2:M:776:LEU:HD11    | 2.50                     | 0.47              |
| 3:N:260:THR:OG1      | 3:N:261:PRO:HD2     | 2.15                     | 0.47              |
| 1:R8:1379:GLN:O      | 1:R8:1380:LYS:C     | 2.56                     | 0.47              |
| 2:M8:417:ARG:HG3     | 8:L8:298:PHE:HD2    | 1.79                     | 0.47              |
| 2:M8:772:PHE:CE1     | 2:M8:776:LEU:HD12   | 2.49                     | 0.47              |
| 3:N8:167:LEU:HD23    | 3:N8:169:SER:HB2    | 1.95                     | 0.47              |
| 1:R16:1428:VAL:HG13  | 1:R16:1431:ARG:HE   | 1.79                     | 0.47              |
| 2:M16:739:TYR:CE1    | 2:M16:798:MET:CE    | 2.97                     | 0.47              |
| 3:N16:116:ILE:HG23   | 3:N16:177:TYR:CZ    | 2.47                     | 0.47              |
| 3:N16:163:ALA:O      | 3:N16:164:PRO:C     | 2.51                     | 0.47              |
| 3:N16:260:THR:OG1    | 3:N16:261:PRO:HD2   | 2.14                     | 0.47              |
| 5:P:12:GLU:CG        | 5:P:78:GLY:H        | 2.28                     | 0.47              |
| 5:P:159:ILE:HD11     | 5:P:214:LEU:HB2     | 1.97                     | 0.47              |
| 7:Q8:235:ILE:HD13    | 7:Q8:243:CYS:CB     | 2.45                     | 0.47              |
| 5:P16:85:ASP:HB2     | 5:P16:86:PRO:HD3    | 1.96                     | 0.47              |
| 5:P16:607:PHE:CG     | 5:P16:629:ARG:NH1   | 2.82                     | 0.47              |
| 9:K:614:PHE:C        | 9:K:683:GLN:HE21    | 2.10                     | 0.47              |
| 9:K:897:LEU:HD22     | 9:K:901:TRP:CZ2     | 2.50                     | 0.47              |
| 9:K:1160:ARG:HH22    | 9:K:1220:ASN:ND2    | 2.11                     | 0.47              |
| 9:K8:1091:ALA:C      | 9:K8:1093:SER:H     | 2.21                     | 0.47              |
| 9:K8:1153:ALA:C      | 9:K8:1220:ASN:ND2   | 2.63                     | 0.47              |
| 9:K8:1249:MET:HG2    | 9:K8:1254:PHE:CZ    | 2.47                     | 0.47              |
| 9:K16:1180:TRP:CG    | 9:K16:1261:MET:HE3  | 2.50                     | 0.47              |
| 10:C16:572:ILE:C     | 10:C16:574:PRO:HD2  | 2.40                     | 0.47              |
| 10:C16:798:VAL:HG12  | 10:C16:802:TRP:CD2  | 2.48                     | 0.47              |
| 10:C16:919:ASP:H     | 10:C16:927:THR:HG21 | 1.79                     | 0.47              |
| 10:C16:1271:PHE:HD1  | 10:C16:1273:GLY:H   | 1.54                     | 0.47              |
| 10:C16:1283:LEU:CD2  | 10:C16:1287:MET:HE2 | 2.45                     | 0.47              |
| 10:C16:1637:PHE:CE1  | 11:A24:136:LEU:CD1  | 2.90                     | 0.47              |
| 10:C24:381:ILE:CG2   | 10:C24:385:TYR:CZ   | 2.97                     | 0.47              |
| 10:C24:386:ASN:O     | 10:C24:449:GLU:OE2  | 2.32                     | 0.47              |
| 10:C24:1133:ILE:CG1  | 10:C24:1152:LYS:HD2 | 2.43                     | 0.47              |
| 10:C24:1337:LEU:HD23 | 11:A40:126:ARG:HH11 | 1.80                     | 0.47              |
| 10:C24:1394:GLN:NE2  | 24:D24:1158:SER:HB2 | 2.29                     | 0.47              |
| 10:C24:1424:GLN:HE22 | 10:C24:1478:VAL:CG1 | 2.27                     | 0.47              |
| 10:C24:1616:ILE:O    | 10:C24:1618:SER:N   | 2.46                     | 0.47              |
| 11:A40:455:LEU:HD23  | 11:A40:458:ILE:HD12 | 1.95                     | 0.47              |
| 12:A:131:TYR:CG      | 10:C:1469:HIS:HB2   | 2.50                     | 0.47              |
| 12:A:809:VAL:N       | 12:A:810:PRO:CD     | 2.77                     | 0.47              |
| 13:V:776:LEU:HD22    | 14:W:660:LEU:HD12   | 1.97                     | 0.47              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 14:W:680:ARG:HB3     | 15:J:603:LEU:CD2    | 2.45                     | 0.47              |
| 10:C:979:MET:CE      | 10:C:1028:ILE:CB    | 2.90                     | 0.47              |
| 10:C:1703:ILE:CD1    | 10:C:1741:MET:HE2   | 2.42                     | 0.47              |
| 11:A16:90:PHE:CA     | 18:B:1800:ARG:HH22  | 2.16                     | 0.47              |
| 11:A16:288:HIS:CB    | 11:A16:354:ARG:NH1  | 2.71                     | 0.47              |
| 11:A16:809:VAL:N     | 11:A16:810:PRO:CD   | 2.77                     | 0.47              |
| 11:A32:557:LEU:CD2   | 11:A32:561:ASP:CB   | 2.90                     | 0.47              |
| 18:B:583:ARG:CZ      | 18:B:711:CYS:SG     | 3.03                     | 0.47              |
| 18:B:603:PHE:HB3     | 18:B:619:ARG:CZ     | 2.40                     | 0.47              |
| 18:B:628:VAL:HA      | 18:B:631:LEU:HD12   | 1.95                     | 0.47              |
| 18:B:850:GLU:C       | 18:B:852:THR:H      | 2.23                     | 0.47              |
| 18:B:973:ASP:O       | 18:B:974:SER:C      | 2.52                     | 0.47              |
| 18:B:1094:MET:CE     | 18:B:1145:TRP:CH2   | 2.98                     | 0.47              |
| 18:B:1130:LEU:HD23   | 18:B:1132:TRP:CD1   | 2.46                     | 0.47              |
| 18:B:1161:LEU:HG     | 18:B:1403:ILE:HD13  | 1.96                     | 0.47              |
| 18:B:1360:SER:O      | 18:B:1361:ALA:C     | 2.53                     | 0.47              |
| 18:B:1806:HIS:C      | 18:B:1808:GLY:H     | 2.22                     | 0.47              |
| 18:B8:195:MET:HG2    | 18:B8:199:LEU:HB3   | 1.97                     | 0.47              |
| 18:B8:1424:LEU:HD23  | 18:B8:1490:ILE:CD1  | 2.45                     | 0.47              |
| 18:B8:1439:LYS:HZ1   | 24:D32:1257:ASN:CG  | 2.23                     | 0.47              |
| 19:4:311:PHE:CE2     | 19:4:393:VAL:HG21   | 2.50                     | 0.47              |
| 20:E:31:PHE:HE1      | 20:E:46:PHE:HZ      | 1.62                     | 0.47              |
| 20:E:473:LEU:CD2     | 20:E:480:MET:SD     | 3.01                     | 0.47              |
| 19:48:117:ILE:HG13   | 19:48:150:LEU:CD2   | 2.44                     | 0.47              |
| 19:48:122:GLN:HG2    | 19:48:140:THR:CG2   | 2.43                     | 0.47              |
| 20:E8:434:TRP:CE2    | 24:D40:72:GLU:HB2   | 2.46                     | 0.47              |
| 20:E8:440:VAL:O      | 20:E8:442:LYS:N     | 2.46                     | 0.47              |
| 21:H:253:ARG:NH1     | 23:J32:614:ASP:OD1  | 2.47                     | 0.47              |
| 21:H24:255:LEU:HD21  | 22:I24:265:THR:HG21 | 1.97                     | 0.47              |
| 21:H24:322:LEU:CD2   | 22:I24:300:LEU:HD11 | 2.44                     | 0.47              |
| 22:I24:300:LEU:HD22  | 23:J24:689:LEU:CD2  | 2.42                     | 0.47              |
| 24:D:1099:ARG:NH1    | 24:D:1149:VAL:CG1   | 2.77                     | 0.47              |
| 10:C32:768:ARG:HH22  | 10:C32:775:LYS:HG2  | 1.67                     | 0.47              |
| 10:C32:847:ARG:HH22  | 10:C32:912:THR:H    | 1.62                     | 0.47              |
| 10:C32:1061:ASN:O    | 10:C32:1063:PRO:CD  | 2.62                     | 0.47              |
| 10:C32:1616:ILE:O    | 10:C32:1618:SER:N   | 2.46                     | 0.47              |
| 10:C32:1708:ARG:HH21 | 10:C32:1733:ARG:CZ  | 2.27                     | 0.47              |
| 10:C32:1821:VAL:CG1  | 12:A48:144:LYS:CE   | 2.93                     | 0.47              |
| 12:A48:354:ARG:HA    | 12:A48:452:TRP:CE2  | 2.50                     | 0.47              |
| 12:A48:809:VAL:N     | 12:A48:810:PRO:CD   | 2.77                     | 0.47              |
| 1:R:1335:ILE:CG1     | 10:C:1170:VAL:HG11  | 2.44                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R:1434:VAL:HG21    | 3:N:151:VAL:O        | 2.15                     | 0.47              |
| 2:M:762:LEU:CD1      | 2:M:813:ASN:ND2      | 2.77                     | 0.47              |
| 3:N:236:GLY:HA2      | 3:N:260:THR:O        | 2.15                     | 0.47              |
| 1:R8:634:ARG:CD      | 4:T8:160:HIS:HE1     | 2.03                     | 0.47              |
| 2:M8:820:LEU:CD2     | 4:T8:656:TRP:CZ2     | 2.98                     | 0.47              |
| 3:N8:222:LEU:CD1     | 3:N8:270:THR:HA      | 2.44                     | 0.47              |
| 3:N16:19:MET:CE      | 3:N16:23:GLY:HA2     | 2.40                     | 0.47              |
| 3:N16:26:ILE:HD11    | 3:N16:40:VAL:HG21    | 1.95                     | 0.47              |
| 5:P8:12:GLU:CG       | 5:P8:78:GLY:H        | 2.28                     | 0.47              |
| 7:Q8:219:GLY:C       | 7:Q8:221:TRP:N       | 2.73                     | 0.47              |
| 6:O16:173:VAL:CG2    | 6:O16:189:LEU:CD1    | 2.85                     | 0.47              |
| 9:K8:897:LEU:HD22    | 9:K8:901:TRP:CZ2     | 2.50                     | 0.47              |
| 10:C16:319:ALA:HA    | 10:C16:392:LEU:HD11  | 1.97                     | 0.47              |
| 10:C16:573:GLU:N     | 10:C16:574:PRO:HD2   | 2.30                     | 0.47              |
| 10:C16:966:CYS:HA    | 10:C16:1025:LEU:HD13 | 1.93                     | 0.47              |
| 10:C16:1469:HIS:HB2  | 11:A24:131:TYR:CG    | 2.50                     | 0.47              |
| 10:C16:1703:ILE:CD1  | 10:C16:1741:MET:HE2  | 2.42                     | 0.47              |
| 10:C16:1708:ARG:HH21 | 10:C16:1733:ARG:CZ   | 2.27                     | 0.47              |
| 10:C16:1708:ARG:CB   | 10:C16:1730:ILE:CD1  | 2.93                     | 0.47              |
| 11:A24:155:SER:OG    | 11:A24:555:HIS:CE1   | 2.67                     | 0.47              |
| 11:A24:820:LEU:HD22  | 11:A24:830:ILE:HG23  | 1.96                     | 0.47              |
| 10:C24:265:PHE:CE1   | 10:C24:389:LEU:HD12  | 2.50                     | 0.47              |
| 10:C24:1488:ILE:HG21 | 10:C24:1525:VAL:HG13 | 1.96                     | 0.47              |
| 10:C24:1703:ILE:CD1  | 10:C24:1741:MET:HE2  | 2.42                     | 0.47              |
| 13:V:773:LEU:HD21    | 15:J:582:LEU:CD1     | 2.45                     | 0.47              |
| 14:W:656:GLN:HE21    | 15:J:579:ARG:HB2     | 1.76                     | 0.47              |
| 10:C:168:ARG:HH12    | 10:C:228:ARG:C       | 2.23                     | 0.47              |
| 10:C:798:VAL:HG12    | 10:C:802:TRP:CD2     | 2.49                     | 0.47              |
| 10:C:1708:ARG:CB     | 10:C:1730:ILE:CD1    | 2.93                     | 0.47              |
| 10:C8:394:SER:CA     | 10:C8:458:VAL:HG11   | 2.44                     | 0.47              |
| 10:C8:572:ILE:C      | 10:C8:574:PRO:HD2    | 2.40                     | 0.47              |
| 11:A16:140:TRP:HB2   | 18:B:1832:LYS:NZ     | 2.30                     | 0.47              |
| 11:A16:305:LEU:HD12  | 11:A16:317:ALA:HB2   | 1.96                     | 0.47              |
| 11:A32:354:ARG:HA    | 11:A32:452:TRP:CE2   | 2.50                     | 0.47              |
| 18:B:366:ALA:HB1     | 18:B:369:SER:OG      | 2.15                     | 0.47              |
| 18:B:1342:LEU:CD2    | 18:B:1406:ALA:HB3    | 2.42                     | 0.47              |
| 18:B:1649:SER:OG     | 18:B:1653:LEU:HD12   | 2.14                     | 0.47              |
| 18:B8:508:ALA:O      | 18:B8:510:GLN:N      | 2.48                     | 0.47              |
| 18:B8:1094:MET:CE    | 18:B8:1145:TRP:CH2   | 2.98                     | 0.47              |
| 19:4:23:GLN:O        | 19:4:24:ASN:OD1      | 2.33                     | 0.47              |
| 20:E:197:LEU:CD2     | 20:E:201:LEU:HD13    | 2.45                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 19:48:59:GLY:C      | 19:48:61:GLU:N      | 2.73                     | 0.47              |
| 20:E8:197:LEU:CD2   | 20:E8:201:LEU:HD13  | 2.45                     | 0.47              |
| 20:E8:353:ILE:CD1   | 20:E8:413:PHE:O     | 2.63                     | 0.47              |
| 21:H:255:LEU:HD21   | 22:I:265:THR:HG21   | 1.97                     | 0.47              |
| 21:H8:215:ARG:NH1   | 21:H8:219:LYS:HZ2   | 2.13                     | 0.47              |
| 22:I8:203:GLN:N     | 22:I8:204:PRO:HD2   | 2.29                     | 0.47              |
| 21:H16:145:TYR:HB3  | 21:H16:148:GLN:HE21 | 1.79                     | 0.47              |
| 10:C32:667:ILE:HG22 | 10:C32:670:GLU:H    | 1.80                     | 0.47              |
| 1:R:1188:TYR:OH     | 24:D:1459:LEU:HB3   | 2.14                     | 0.47              |
| 1:R:1424:LYS:NZ     | 6:O:134:ARG:NH2     | 2.57                     | 0.47              |
| 2:M:625:HIS:CD2     | 3:N:225:PRO:CB      | 2.98                     | 0.47              |
| 1:R8:1434:VAL:HG21  | 3:N8:151:VAL:O      | 2.15                     | 0.47              |
| 2:M16:820:LEU:CD2   | 4:T16:656:TRP:CZ2   | 2.98                     | 0.47              |
| 2:M16:851:LEU:CD2   | 4:T16:653:GLN:CG    | 2.85                     | 0.47              |
| 5:P:25:LEU:HD21     | 6:O:322:GLU:OE2     | 2.15                     | 0.47              |
| 5:P:247:GLU:N       | 5:P:247:GLU:CD      | 2.70                     | 0.47              |
| 5:P:285:PRO:HG2     | 5:P:310:ARG:HA      | 1.95                     | 0.47              |
| 5:P8:25:LEU:HD21    | 6:O8:322:GLU:OE2    | 2.15                     | 0.47              |
| 5:P8:499:TYR:CE1    | 5:P8:527:LYS:HD3    | 2.49                     | 0.47              |
| 6:O8:173:VAL:CG2    | 6:O8:189:LEU:CD1    | 2.85                     | 0.47              |
| 6:O16:180:GLY:O     | 6:O16:182:GLU:N     | 2.47                     | 0.47              |
| 8:L8:605:MET:CG     | 8:L8:631:LEU:CD1    | 2.92                     | 0.47              |
| 9:K8:1051:GLU:O     | 9:K8:1053:MET:N     | 2.48                     | 0.47              |
| 10:C16:265:PHE:CE1  | 10:C16:389:LEU:HD12 | 2.50                     | 0.47              |
| 10:C24:664:ASN:O    | 10:C24:668:ALA:N    | 2.42                     | 0.47              |
| 11:A40:820:LEU:HD22 | 11:A40:830:ILE:HG23 | 1.96                     | 0.47              |
| 12:A:465:SER:C      | 12:A:467:SER:N      | 2.72                     | 0.47              |
| 13:V:828:ASN:HD21   | 14:W:705:HIS:CE1    | 2.32                     | 0.47              |
| 10:C:144:ASP:CB     | 10:C:147:LEU:HD12   | 2.44                     | 0.47              |
| 10:C8:643:LEU:CB    | 10:C8:679:ARG:HH22  | 2.05                     | 0.47              |
| 10:C8:1069:TYR:HA   | 10:C8:1070:PRO:HD3  | 1.65                     | 0.47              |
| 10:C8:1616:ILE:O    | 10:C8:1618:SER:N    | 2.46                     | 0.47              |
| 11:A32:36:ASN:HD22  | 22:I24:293:LYS:HZ3  | 1.56                     | 0.47              |
| 11:A32:526:GLY:C    | 11:A32:528:GLY:H    | 2.23                     | 0.47              |
| 18:B:907:SER:OG     | 18:B:910:TYR:HB2    | 2.15                     | 0.47              |
| 18:B:968:PHE:CD1    | 18:B:999:LEU:HD12   | 2.50                     | 0.47              |
| 18:B:1911:LEU:CB    | 18:B:1960:LEU:HD12  | 2.45                     | 0.47              |
| 18:B8:7:VAL:HG12    | 18:B8:11:LEU:HD12   | 1.97                     | 0.47              |
| 18:B8:583:ARG:CZ    | 18:B8:711:CYS:SG    | 3.03                     | 0.47              |
| 18:B8:904:ALA:HB2   | 18:B8:917:PHE:CZ    | 2.49                     | 0.47              |
| 18:B8:1496:GLY:CA   | 24:D32:1302:ASP:OD2 | 2.63                     | 0.47              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 19:4:444:HIS:C      | 19:4:446:LEU:H       | 2.23                     | 0.47              |
| 20:E:353:ILE:CD1    | 20:E:413:PHE:O       | 2.63                     | 0.47              |
| 22:I:196:VAL:HG22   | 23:J32:620:MET:HE3   | 1.96                     | 0.47              |
| 21:H8:228:LEU:CD2   | 23:J8:592:VAL:CG1    | 2.92                     | 0.47              |
| 24:D32:642:VAL:CG2  | 24:D40:631:ARG:NH2   | 2.64                     | 0.47              |
| 24:D40:749:ARG:NH1  | 24:D40:964:LEU:HA    | 2.29                     | 0.47              |
| 10:C32:168:ARG:HH12 | 10:C32:228:ARG:C     | 2.23                     | 0.47              |
| 10:C32:1599:ASP:CG  | 10:C32:1604:VAL:HG23 | 2.39                     | 0.47              |
| 10:C32:1610:MET:HG2 | 10:C32:1614:LEU:HD12 | 1.97                     | 0.47              |
| 12:A48:526:GLY:C    | 12:A48:528:GLY:H     | 2.23                     | 0.47              |
| 12:A48:778:ILE:HD13 | 12:A48:816:ALA:HB2   | 1.95                     | 0.47              |
| 1:R:979:GLN:CB      | 24:D:1438:ALA:HB3    | 2.45                     | 0.47              |
| 1:R:1124:TRP:CH2    | 4:T:669:PRO:CG       | 2.96                     | 0.47              |
| 2:M:250:LEU:HD23    | 2:M:287:TYR:CG       | 2.50                     | 0.47              |
| 2:M:328:THR:O       | 2:M:329:GLU:C        | 2.53                     | 0.47              |
| 3:N:202:CYS:O       | 3:N:204:PRO:O        | 2.33                     | 0.47              |
| 1:R8:1472:HIS:CE1   | 1:R8:1476:LEU:HD11   | 2.50                     | 0.47              |
| 2:M16:772:PHE:CE1   | 2:M16:776:LEU:HD12   | 2.49                     | 0.47              |
| 5:P:507:GLN:HE21    | 7:Q:136:ARG:NH2      | 2.13                     | 0.47              |
| 5:P16:25:LEU:HD21   | 6:O16:322:GLU:OE2    | 2.15                     | 0.47              |
| 7:Q16:219:GLY:C     | 7:Q16:221:TRP:N      | 2.73                     | 0.47              |
| 8:L16:1038:MET:CE   | 8:L16:1054:HIS:NE2   | 2.77                     | 0.47              |
| 9:K8:975:MET:HA     | 9:K8:985:PHE:CE1     | 2.48                     | 0.47              |
| 9:K16:894:LYS:CE    | 9:K16:1057:GLU:HB3   | 2.37                     | 0.47              |
| 10:C16:16:LEU:HD22  | 10:C16:139:ARG:HH12  | 1.80                     | 0.47              |
| 10:C16:803:ARG:HH21 | 10:C16:808:PRO:CG    | 2.28                     | 0.47              |
| 10:C16:1137:SER:HB3 | 10:C16:1143:LEU:HD12 | 1.96                     | 0.47              |
| 11:A24:711:ARG:HG2  | 11:A24:713:ASP:OD1   | 2.14                     | 0.47              |
| 10:C24:229:PRO:HG2  | 10:C24:270:THR:CG2   | 2.45                     | 0.47              |
| 10:C24:572:ILE:C    | 10:C24:574:PRO:HD2   | 2.40                     | 0.47              |
| 10:C24:729:SER:C    | 10:C24:731:GLN:N     | 2.73                     | 0.47              |
| 10:C24:803:ARG:HH21 | 10:C24:808:PRO:CG    | 2.28                     | 0.47              |
| 10:C24:847:ARG:HH22 | 10:C24:912:THR:H     | 1.62                     | 0.47              |
| 10:C24:919:ASP:H    | 10:C24:927:THR:HG21  | 1.79                     | 0.47              |
| 11:A40:259:ILE:HG23 | 11:A40:276:LEU:HD22  | 1.96                     | 0.47              |
| 11:A40:354:ARG:HA   | 11:A40:452:TRP:CE2   | 2.49                     | 0.47              |
| 11:A40:557:LEU:CD2  | 11:A40:561:ASP:CB    | 2.90                     | 0.47              |
| 13:V:836:LEU:CD2    | 14:W:716:PHE:CE1     | 2.98                     | 0.47              |
| 13:V:840:ARG:NH2    | 14:W:719:GLU:OE1     | 2.48                     | 0.47              |
| 13:V:854:LEU:HD21   | 14:W:734:SER:CB      | 2.41                     | 0.47              |
| 15:J:688:PRO:O      | 15:J:692:VAL:HG23    | 2.15                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:847:ARG:HH22    | 10:C:912:THR:H       | 1.63                     | 0.47              |
| 10:C:1283:LEU:CD2    | 10:C:1287:MET:HE2    | 2.45                     | 0.47              |
| 10:C8:1137:SER:HB3   | 10:C8:1143:LEU:HD12  | 1.95                     | 0.47              |
| 11:A16:90:PHE:CG     | 18:B:1788:ILE:CD1    | 2.86                     | 0.47              |
| 11:A16:711:ARG:HG2   | 11:A16:713:ASP:OD1   | 2.14                     | 0.47              |
| 11:A32:557:LEU:HD23  | 11:A32:561:ASP:CB    | 2.44                     | 0.47              |
| 18:B:195:MET:HG2     | 18:B:199:LEU:HB3     | 1.97                     | 0.47              |
| 18:B:618:VAL:HG11    | 18:B:621:VAL:HG21    | 1.97                     | 0.47              |
| 18:B:1571:HIS:CG     | 24:D16:1407:PHE:HB2  | 2.06                     | 0.47              |
| 18:B8:475:GLU:O      | 18:B8:479:PRO:HG2    | 2.14                     | 0.47              |
| 18:B8:1298:GLN:HG2   | 18:B8:1303:ILE:HD12  | 1.96                     | 0.47              |
| 22:I24:196:VAL:HG22  | 23:J24:620:MET:HE3   | 1.97                     | 0.47              |
| 21:H16:322:LEU:CD2   | 22:I16:300:LEU:HD11  | 2.44                     | 0.47              |
| 22:I16:203:GLN:N     | 22:I16:204:PRO:HD2   | 2.29                     | 0.47              |
| 24:D24:1330:ARG:HG3  | 24:D24:1331:ASP:N    | 2.29                     | 0.47              |
| 10:C32:1017:HIS:CD2  | 10:C32:1139:ARG:HD3  | 2.50                     | 0.47              |
| 10:C32:1137:SER:HB3  | 10:C32:1143:LEU:HD12 | 1.96                     | 0.47              |
| 10:C32:1293:THR:HG23 | 10:C32:1369:LEU:HD13 | 1.96                     | 0.47              |
| 12:A48:212:LYS:HE3   | 12:A48:585:MET:HE3   | 1.76                     | 0.47              |
| 2:M16:411:ILE:HG21   | 8:L16:397:CYS:SG     | 2.55                     | 0.46              |
| 3:N16:208:LYS:HB2    | 3:N16:241:TRP:HH2    | 1.80                     | 0.46              |
| 6:O:119:ARG:NH2      | 6:O:182:GLU:CA       | 2.57                     | 0.46              |
| 7:Q:33:ARG:HH22      | 7:Q:345:ASP:HB3      | 1.78                     | 0.46              |
| 5:P8:175:MET:CE      | 5:P8:433:LEU:HD23    | 2.43                     | 0.46              |
| 9:K:1113:ILE:HD13    | 9:K:1136:CYS:SG      | 2.55                     | 0.46              |
| 9:K8:879:CYS:HB3     | 9:K8:900:TYR:CE2     | 2.50                     | 0.46              |
| 10:C16:144:ASP:CB    | 10:C16:147:LEU:HD12  | 2.44                     | 0.46              |
| 10:C16:1337:LEU:HD23 | 11:A24:126:ARG:HH11  | 1.80                     | 0.46              |
| 10:C16:1610:MET:HG2  | 10:C16:1614:LEU:HD12 | 1.97                     | 0.46              |
| 10:C24:238:TYR:CZ    | 10:C24:313:ILE:HD13  | 2.50                     | 0.46              |
| 10:C:265:PHE:CE1     | 10:C:389:LEU:HD12    | 2.50                     | 0.46              |
| 10:C8:1610:MET:HG2   | 10:C8:1614:LEU:HD12  | 1.97                     | 0.46              |
| 11:A32:72:ILE:HD13   | 21:H24:348:ALA:CB    | 2.45                     | 0.46              |
| 18:B:567:LEU:HD13    | 18:B:627:SER:HB3     | 1.96                     | 0.46              |
| 18:B:1660:SER:HA     | 18:B:1724:MET:HE1    | 1.96                     | 0.46              |
| 18:B8:907:SER:OG     | 18:B8:910:TYR:HB2    | 2.15                     | 0.46              |
| 18:B8:968:PHE:CD1    | 18:B8:999:LEU:HD12   | 2.50                     | 0.46              |
| 18:B8:1733:SER:O     | 18:B8:1871:GLN:NE2   | 2.48                     | 0.46              |
| 21:H24:363:MET:O     | 21:H24:367:VAL:HG23  | 2.15                     | 0.46              |
| 21:H16:363:MET:O     | 21:H16:367:VAL:HG23  | 2.15                     | 0.46              |
| 24:D40:274:MET:HE3   | 24:D40:321:SER:CB    | 2.42                     | 0.46              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 24:D40:865:VAL:HG21  | 24:D40:932:ARG:HH12 | 1.80                     | 0.46              |
| 10:C32:764:ILE:HD13  | 10:C32:781:VAL:HG21 | 1.94                     | 0.46              |
| 10:C32:1507:LEU:C    | 10:C32:1509:SER:N   | 2.67                     | 0.46              |
| 1:R8:1124:TRP:HH2    | 4:T8:669:PRO:CA     | 2.28                     | 0.46              |
| 2:M8:739:TYR:CE1     | 2:M8:798:MET:CE     | 2.97                     | 0.46              |
| 3:N8:236:GLY:HA2     | 3:N8:260:THR:O      | 2.15                     | 0.46              |
| 1:R16:1124:TRP:HH2   | 4:T16:669:PRO:CA    | 2.28                     | 0.46              |
| 1:R16:1438:TRP:NE1   | 3:N16:58:PRO:HG2    | 2.31                     | 0.46              |
| 5:P8:507:GLN:HE21    | 7:Q8:136:ARG:NH2    | 2.13                     | 0.46              |
| 5:P16:34:SER:OG      | 5:P16:55:ARG:NH2    | 2.48                     | 0.46              |
| 8:L8:1081:MET:HG3    | 9:K8:1087:ALA:HB2   | 1.97                     | 0.46              |
| 9:K:1028:GLN:OE1     | 9:K:1040:THR:OG1    | 2.31                     | 0.46              |
| 9:K:1277:ALA:O       | 9:K:1278:GLU:C      | 2.56                     | 0.46              |
| 9:K8:601:VAL:CG1     | 9:K8:673:SER:HB3    | 2.38                     | 0.46              |
| 10:C16:123:TRP:CZ2   | 10:C16:127:ARG:HD2  | 2.50                     | 0.46              |
| 10:C16:238:TYR:CZ    | 10:C16:313:ILE:HD13 | 2.50                     | 0.46              |
| 10:C16:1188:TRP:CZ2  | 10:C16:1192:ARG:HD2 | 2.51                     | 0.46              |
| 10:C16:1547:LYS:HE2  | 24:D8:1405:GLY:HA2  | 1.97                     | 0.46              |
| 11:A24:72:ILE:HD13   | 21:H8:348:ALA:HA    | 1.95                     | 0.46              |
| 10:C24:123:TRP:CZ2   | 10:C24:127:ARG:HD2  | 2.50                     | 0.46              |
| 10:C24:168:ARG:HH12  | 10:C24:228:ARG:C    | 2.23                     | 0.46              |
| 10:C24:1002:LEU:HD11 | 10:C24:1016:LEU:CD2 | 2.45                     | 0.46              |
| 11:A40:20:LEU:HD11   | 21:H16:346:THR:HG23 | 1.91                     | 0.46              |
| 11:A40:72:ILE:HD13   | 21:H16:348:ALA:CB   | 2.45                     | 0.46              |
| 12:A:354:ARG:HA      | 12:A:452:TRP:CE2    | 2.50                     | 0.46              |
| 10:C:1188:TRP:CZ2    | 10:C:1192:ARG:HD2   | 2.51                     | 0.46              |
| 10:C8:1002:LEU:HD11  | 10:C8:1016:LEU:CD2  | 2.45                     | 0.46              |
| 10:C8:1708:ARG:HH21  | 10:C8:1733:ARG:CZ   | 2.27                     | 0.46              |
| 11:A32:703:ALA:CA    | 24:D32:1398:ARG:CD  | 2.84                     | 0.46              |
| 18:B:729:LEU:CD1     | 18:B:1196:MET:SD    | 3.03                     | 0.46              |
| 18:B:1161:LEU:CD2    | 18:B:1403:ILE:HD12  | 2.41                     | 0.46              |
| 18:B8:1515:LEU:HD21  | 18:B8:1563:PHE:CB   | 2.45                     | 0.46              |
| 18:B8:1668:PHE:CE2   | 18:B8:1731:PHE:CD2  | 3.00                     | 0.46              |
| 18:B8:1714:MET:O     | 18:B8:1718:ASP:HB2  | 2.15                     | 0.46              |
| 18:B8:1749:LEU:C     | 18:B8:1781:VAL:HG13 | 2.37                     | 0.46              |
| 19:48:16:ASN:O       | 19:48:17:ARG:HB2    | 2.15                     | 0.46              |
| 19:48:311:PHE:CE2    | 19:48:393:VAL:HG21  | 2.50                     | 0.46              |
| 19:48:417:ASP:OD1    | 19:48:423:PRO:HB3   | 2.15                     | 0.46              |
| 20:E8:24:ILE:HB      | 20:E8:25:PRO:CD     | 2.45                     | 0.46              |
| 20:E8:123:CYS:SG     | 20:E8:135:ILE:CG2   | 2.99                     | 0.46              |
| 22:I8:196:VAL:HG22   | 23:J8:620:MET:HE3   | 1.97                     | 0.46              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 22:I8:333:ARG:NH2    | 22:I8:350:PHE:HB2   | 2.30                     | 0.46              |
| 21:H24:326:GLY:C     | 21:H24:328:THR:H    | 2.22                     | 0.46              |
| 10:C32:1283:LEU:CD2  | 10:C32:1287:MET:HE2 | 2.45                     | 0.46              |
| 10:C32:1352:GLN:HE22 | 10:C32:1357:LEU:CD1 | 2.29                     | 0.46              |
| 12:A48:198:PRO:CB    | 12:A48:200:HIS:HE1  | 2.24                     | 0.46              |
| 1:R:1139:ARG:CD      | 1:R:1157:ARG:NH2    | 2.66                     | 0.46              |
| 3:N8:208:LYS:HB2     | 3:N8:241:TRP:HH2    | 1.80                     | 0.46              |
| 1:R16:1445:GLU:HG3   | 2:M16:168:LEU:HD12  | 1.96                     | 0.46              |
| 1:R16:1472:HIS:CE1   | 1:R16:1476:LEU:HD11 | 2.49                     | 0.46              |
| 2:M16:401:ARG:HH21   | 8:L16:381:GLU:HB3   | 1.66                     | 0.46              |
| 3:N16:158:TRP:CZ2    | 3:N16:179:LEU:HD21  | 2.48                     | 0.46              |
| 5:P8:85:ASP:HB2      | 5:P8:86:PRO:HD3     | 1.97                     | 0.46              |
| 5:P16:503:VAL:HG11   | 5:P16:528:LEU:HD22  | 1.98                     | 0.46              |
| 9:K8:700:MET:HE1     | 9:K8:767:LEU:HD13   | 1.95                     | 0.46              |
| 9:K8:727:ASP:C       | 9:K8:729:VAL:N      | 2.73                     | 0.46              |
| 9:K8:806:LEU:HD12    | 9:K8:874:VAL:CG1    | 2.44                     | 0.46              |
| 9:K8:1180:TRP:CZ2    | 9:K8:1206:LEU:CD1   | 2.92                     | 0.46              |
| 9:K16:975:MET:HG2    | 9:K16:985:PHE:CE1   | 2.51                     | 0.46              |
| 10:C16:229:PRO:HG2   | 10:C16:270:THR:CG2  | 2.45                     | 0.46              |
| 10:C16:1278:ASP:OD1  | 21:H:282:GLU:HG2    | 2.16                     | 0.46              |
| 11:A24:354:ARG:HA    | 11:A24:452:TRP:CE2  | 2.50                     | 0.46              |
| 10:C24:168:ARG:HH22  | 10:C24:227:ASP:C    | 2.23                     | 0.46              |
| 10:C24:277:SER:O     | 10:C24:280:SER:N    | 2.35                     | 0.46              |
| 10:C24:319:ALA:HA    | 10:C24:392:LEU:HD11 | 1.98                     | 0.46              |
| 10:C24:1352:GLN:HE22 | 10:C24:1357:LEU:CD1 | 2.29                     | 0.46              |
| 10:C24:1708:ARG:HH21 | 10:C24:1733:ARG:CZ  | 2.27                     | 0.46              |
| 10:C24:1708:ARG:CB   | 10:C24:1730:ILE:CD1 | 2.93                     | 0.46              |
| 13:V:783:TRP:CZ2     | 14:W:671:GLU:CB     | 2.98                     | 0.46              |
| 14:W:698:LEU:HD21    | 15:J:621:GLU:HA     | 1.96                     | 0.46              |
| 10:C:62:ILE:HD13     | 10:C:95:VAL:HG21    | 1.97                     | 0.46              |
| 10:C:803:ARG:HH21    | 10:C:808:PRO:CG     | 2.28                     | 0.46              |
| 10:C:837:ARG:NH2     | 10:C:890:ASP:O      | 2.49                     | 0.46              |
| 10:C8:123:TRP:CZ2    | 10:C8:127:ARG:HD2   | 2.50                     | 0.46              |
| 10:C8:238:TYR:CZ     | 10:C8:313:ILE:HD13  | 2.51                     | 0.46              |
| 10:C8:453:LEU:HD22   | 10:C8:459:LEU:HD21  | 0.51                     | 0.46              |
| 10:C8:758:GLN:HE21   | 10:C8:819:GLN:CG    | 2.24                     | 0.46              |
| 10:C8:1283:LEU:CD2   | 10:C8:1287:MET:HE2  | 2.45                     | 0.46              |
| 10:C8:1337:LEU:HD23  | 16:A8:126:ARG:HH11  | 1.80                     | 0.46              |
| 11:A16:782:PRO:C     | 11:A16:783:PHE:CG   | 2.93                     | 0.46              |
| 18:B:499:ILE:HD11    | 18:B:545:VAL:CG2    | 2.41                     | 0.46              |
| 18:B:508:ALA:O       | 18:B:510:GLN:N      | 2.48                     | 0.46              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B:1098:MET:HE1    | 18:B:1142:PHE:CB    | 2.45                     | 0.46              |
| 18:B:1749:LEU:C      | 18:B:1781:VAL:HG13  | 2.36                     | 0.46              |
| 18:B8:615:GLU:C      | 18:B8:617:ASP:N     | 2.73                     | 0.46              |
| 19:4:16:ASN:O        | 19:4:17:ARG:HB2     | 2.15                     | 0.46              |
| 20:E8:440:VAL:C      | 20:E8:442:LYS:N     | 2.74                     | 0.46              |
| 21:H:217:ARG:HH21    | 23:J32:586:GLU:CD   | 2.23                     | 0.46              |
| 21:H8:267:LYS:HZ3    | 23:J8:631:GLU:CD    | 1.98                     | 0.46              |
| 23:J8:686:MET:CE     | 23:J8:694:ARG:HH21  | 2.10                     | 0.46              |
| 21:H24:136:TYR:CE2   | 23:J24:554:LEU:HD13 | 2.49                     | 0.46              |
| 21:H16:228:LEU:CD2   | 23:J16:592:VAL:CG1  | 2.92                     | 0.46              |
| 22:I16:333:ARG:NH2   | 22:I16:350:PHE:HB2  | 2.30                     | 0.46              |
| 24:D16:552:VAL:HG21  | 24:D16:592:ILE:HD11 | 1.97                     | 0.46              |
| 24:D16:1099:ARG:O    | 24:D16:1099:ARG:CG  | 2.63                     | 0.46              |
| 24:D40:552:VAL:HG21  | 24:D40:592:ILE:HD11 | 1.97                     | 0.46              |
| 10:C32:238:TYR:CZ    | 10:C32:313:ILE:HD13 | 2.50                     | 0.46              |
| 12:A48:388:VAL:CG1   | 12:A48:392:SER:HB2  | 2.46                     | 0.46              |
| 1:R:1428:VAL:HB      | 6:O:165:LYS:HZ2     | 1.79                     | 0.46              |
| 2:M:762:LEU:CD2      | 2:M:813:ASN:HD22    | 2.29                     | 0.46              |
| 2:M8:358:LEU:N       | 2:M8:359:PRO:CD     | 2.79                     | 0.46              |
| 3:N16:236:GLY:HA2    | 3:N16:260:THR:O     | 2.15                     | 0.46              |
| 5:P:34:SER:OG        | 5:P:55:ARG:NH2      | 2.48                     | 0.46              |
| 5:P:220:GLU:OE2      | 5:P:232:ARG:NH2     | 2.49                     | 0.46              |
| 5:P:398:LYS:CD       | 5:P:426:MET:CE      | 2.94                     | 0.46              |
| 5:P:592:SER:HG       | 5:P:598:LEU:CD1     | 2.07                     | 0.46              |
| 5:P8:34:SER:OG       | 5:P8:55:ARG:NH2     | 2.48                     | 0.46              |
| 6:O8:282:GLU:HB2     | 6:O8:284:TRP:CE2    | 2.49                     | 0.46              |
| 6:O16:5:MET:CE       | 6:O16:46:PHE:CE2    | 2.99                     | 0.46              |
| 9:K:850:LEU:HD11     | 9:K:864:ILE:HG22    | 1.96                     | 0.46              |
| 9:K:994:TYR:HD2      | 9:K:1023:LEU:CD1    | 2.23                     | 0.46              |
| 9:K:1039:ASP:CG      | 9:K:1096:LYS:HZ1    | 2.16                     | 0.46              |
| 9:K:1048:GLN:HB3     | 9:K:1049:ASP:H      | 1.55                     | 0.46              |
| 9:K8:798:LEU:HB3     | 9:K8:842:ILE:HD11   | 1.97                     | 0.46              |
| 10:C16:54:ARG:HE     | 10:C16:81:LEU:HD22  | 1.80                     | 0.46              |
| 10:C16:705:TYR:O     | 10:C16:794:LYS:NZ   | 2.43                     | 0.46              |
| 10:C16:1352:GLN:HE22 | 10:C16:1357:LEU:CD1 | 2.29                     | 0.46              |
| 11:A24:691:ALA:HA    | 24:D8:1397:THR:HG21 | 1.97                     | 0.46              |
| 10:C24:16:LEU:HD22   | 10:C24:139:ARG:HH12 | 1.81                     | 0.46              |
| 10:C24:453:LEU:HD22  | 10:C24:459:LEU:HD21 | 0.51                     | 0.46              |
| 10:C24:573:GLU:N     | 10:C24:574:PRO:HD2  | 2.30                     | 0.46              |
| 10:C24:1282:CYS:HA   | 10:C24:1738:MET:CE  | 2.41                     | 0.46              |
| 10:C24:1469:HIS:HB2  | 11:A40:131:TYR:CG   | 2.50                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 11:A40:51:THR:CG2   | 22:I16:317:HIS:HB2 | 2.42                     | 0.46              |
| 11:A40:782:PRO:C    | 11:A40:783:PHE:CG  | 2.93                     | 0.46              |
| 13:V:787:ILE:HD11   | 15:J:592:VAL:CG1   | 2.44                     | 0.46              |
| 13:V:847:ASN:ND2    | 14:W:723:TYR:CE1   | 2.73                     | 0.46              |
| 10:C:229:PRO:HG2    | 10:C:270:THR:CG2   | 2.45                     | 0.46              |
| 10:C:238:TYR:CZ     | 10:C:313:ILE:HD13  | 2.51                     | 0.46              |
| 10:C:319:ALA:HA     | 10:C:392:LEU:HD11  | 1.97                     | 0.46              |
| 10:C:1061:ASN:O     | 10:C:1063:PRO:CD   | 2.62                     | 0.46              |
| 10:C:1164:VAL:HG13  | 10:C:1167:PHE:HE2  | 1.81                     | 0.46              |
| 10:C8:229:PRO:HG2   | 10:C8:270:THR:CG2  | 2.45                     | 0.46              |
| 10:C8:573:GLU:OE1   | 10:C8:617:TYR:OH   | 2.32                     | 0.46              |
| 10:C8:1285:VAL:CB   | 10:C8:1738:MET:CE  | 2.85                     | 0.46              |
| 10:C8:1469:HIS:HB2  | 16:A8:131:TYR:CG   | 2.50                     | 0.46              |
| 10:C8:1654:LEU:HD22 | 10:C8:1670:PRO:O   | 2.16                     | 0.46              |
| 11:A16:326:TYR:CD1  | 17:F8:77:TYR:HB3   | 2.13                     | 0.46              |
| 11:A16:465:SER:C    | 11:A16:467:SER:N   | 2.72                     | 0.46              |
| 11:A16:526:GLY:C    | 11:A16:528:GLY:H   | 2.23                     | 0.46              |
| 11:A32:154:ILE:CG2  | 18:B8:1851:VAL:CG2 | 2.94                     | 0.46              |
| 18:B:402:ILE:HG12   | 18:B:407:ILE:HD11  | 1.96                     | 0.46              |
| 18:B:817:CYS:CB     | 18:B:885:ARG:HH12  | 2.08                     | 0.46              |
| 18:B:1733:SER:O     | 18:B:1871:GLN:NE2  | 2.48                     | 0.46              |
| 18:B8:402:ILE:HG12  | 18:B8:407:ILE:HD11 | 1.96                     | 0.46              |
| 18:B8:1175:ALA:HA   | 18:B8:1325:MET:CE  | 2.46                     | 0.46              |
| 19:4:59:GLY:C       | 19:4:61:GLU:N      | 2.73                     | 0.46              |
| 19:4:252:ARG:NH2    | 19:4:286:TRP:O     | 2.47                     | 0.46              |
| 19:4:417:ASP:OD1    | 19:4:423:PRO:HB3   | 2.15                     | 0.46              |
| 20:E:343:THR:CB     | 20:E:344:PRO:HD2   | 2.44                     | 0.46              |
| 20:E8:432:ILE:HG22  | 20:E8:434:TRP:HD1  | 1.80                     | 0.46              |
| 21:H8:217:ARG:HH21  | 23:J8:586:GLU:CD   | 2.23                     | 0.46              |
| 24:D:274:MET:HE3    | 24:D:321:SER:CB    | 2.42                     | 0.46              |
| 10:C32:123:TRP:CZ2  | 10:C32:127:ARG:HD2 | 2.50                     | 0.46              |
| 10:C32:717:GLU:O    | 10:C32:718:HIS:C   | 2.41                     | 0.46              |
| 10:C32:1161:PHE:O   | 10:C32:1162:PRO:C  | 2.55                     | 0.46              |
| 1:R:1124:TRP:CZ2    | 4:T:669:PRO:CD     | 2.99                     | 0.46              |
| 1:R:1438:TRP:NE1    | 3:N:58:PRO:HG2     | 2.31                     | 0.46              |
| 2:M:420:CYS:SG      | 8:L:391:TRP:CH2    | 3.09                     | 0.46              |
| 2:M:820:LEU:CD2     | 4:T:656:TRP:CZ2    | 2.99                     | 0.46              |
| 2:M8:762:LEU:CD1    | 2:M8:813:ASN:ND2   | 2.77                     | 0.46              |
| 5:P:43:TRP:HH2      | 5:P:76:LEU:HD12    | 1.81                     | 0.46              |
| 5:P:281:ILE:HD11    | 5:P:341:MET:CE     | 2.45                     | 0.46              |
| 6:O8:5:MET:CE       | 6:O8:46:PHE:CE2    | 2.99                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K:876:LEU:HD21     | 9:K:904:ARG:HG3      | 1.98                     | 0.46              |
| 9:K:1113:ILE:HD12    | 9:K:1132:LEU:CD2     | 2.45                     | 0.46              |
| 10:C16:729:SER:C     | 10:C16:731:GLN:H     | 2.24                     | 0.46              |
| 10:C16:1488:ILE:CG2  | 10:C16:1525:VAL:HG13 | 2.45                     | 0.46              |
| 10:C16:1488:ILE:HG21 | 10:C16:1525:VAL:HG13 | 1.96                     | 0.46              |
| 10:C16:1821:VAL:CG1  | 11:A24:144:LYS:CE    | 2.93                     | 0.46              |
| 11:A24:782:PRO:C     | 11:A24:783:PHE:CG    | 2.93                     | 0.46              |
| 13:V:817:GLN:C       | 13:V:820:ASP:H       | 2.11                     | 0.46              |
| 10:C:1017:HIS:CD2    | 10:C:1139:ARG:HD3    | 2.50                     | 0.46              |
| 10:C:1488:ILE:CG2    | 10:C:1525:VAL:HG13   | 2.45                     | 0.46              |
| 10:C:1496:PHE:CE1    | 10:C:1498:GLY:O      | 2.69                     | 0.46              |
| 10:C8:54:ARG:HE      | 10:C8:81:LEU:HD22    | 1.80                     | 0.46              |
| 10:C8:470:HIS:CD2    | 10:C8:508:ILE:HD11   | 2.44                     | 0.46              |
| 10:C8:1496:PHE:CE1   | 10:C8:1498:GLY:O     | 2.69                     | 0.46              |
| 10:C8:1708:ARG:CB    | 10:C8:1730:ILE:CD1   | 2.93                     | 0.46              |
| 11:A16:36:ASN:HD22   | 22:I:293:LYS:HZ3     | 1.58                     | 0.46              |
| 11:A16:72:ILE:HD13   | 21:H:348:ALA:CB      | 2.45                     | 0.46              |
| 11:A16:90:PHE:CD2    | 18:B:1788:ILE:HG12   | 2.50                     | 0.46              |
| 11:A16:707:LEU:CA    | 24:D16:1398:ARG:NH2  | 2.78                     | 0.46              |
| 11:A32:104:TYR:CZ    | 18:B8:1102:LYS:NZ    | 2.64                     | 0.46              |
| 11:A32:465:SER:C     | 11:A32:467:SER:N     | 2.72                     | 0.46              |
| 18:B:615:GLU:C       | 18:B:617:ASP:N       | 2.73                     | 0.46              |
| 18:B:1515:LEU:HD21   | 18:B:1563:PHE:CB     | 2.45                     | 0.46              |
| 18:B8:499:ILE:HD11   | 18:B8:545:VAL:CG2    | 2.41                     | 0.46              |
| 18:B8:567:LEU:HD13   | 18:B8:627:SER:HB3    | 1.96                     | 0.46              |
| 18:B8:782:THR:C      | 24:D32:1066:VAL:CG2  | 2.88                     | 0.46              |
| 18:B8:850:GLU:C      | 18:B8:852:THR:H      | 2.23                     | 0.46              |
| 18:B8:1186:LEU:HD21  | 18:B8:1199:VAL:HG13  | 1.97                     | 0.46              |
| 18:B8:1215:PHE:HZ    | 18:B8:1234:MET:SD    | 2.34                     | 0.46              |
| 18:B8:1769:ASN:HA    | 18:B8:1812:GLN:OE1   | 2.15                     | 0.46              |
| 20:E8:447:ILE:HG22   | 20:E8:451:ILE:HB     | 1.96                     | 0.46              |
| 22:I:203:GLN:N       | 22:I:204:PRO:HD2     | 2.29                     | 0.46              |
| 22:I:332:MET:CG      | 23:J32:732:MET:HE1   | 2.46                     | 0.46              |
| 22:I16:196:VAL:HG22  | 23:J16:620:MET:HE3   | 1.97                     | 0.46              |
| 10:C32:1337:LEU:HD23 | 12:A48:126:ARG:HH11  | 1.80                     | 0.46              |
| 10:C32:1469:HIS:HB2  | 12:A48:131:TYR:CG    | 2.50                     | 0.46              |
| 1:R:1335:ILE:HG12    | 10:C:1170:VAL:HG21   | 1.95                     | 0.46              |
| 3:N:128:ASN:HB3      | 3:N:144:ARG:HE       | 1.81                     | 0.46              |
| 5:P:256:HIS:HE1      | 5:P:270:GLU:OE1      | 1.98                     | 0.46              |
| 5:P8:43:TRP:HH2      | 5:P8:76:LEU:HD12     | 1.81                     | 0.46              |
| 5:P8:475:THR:O       | 5:P8:478:ILE:HG12    | 2.16                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:12:GLU:CG      | 5:P16:78:GLY:H       | 2.28                     | 0.46              |
| 5:P16:201:ILE:HD12   | 5:P16:211:TYR:CZ     | 2.51                     | 0.46              |
| 5:P16:475:THR:O      | 5:P16:478:ILE:HG12   | 2.16                     | 0.46              |
| 9:K8:584:SER:CB      | 9:K8:622:VAL:HG21    | 2.42                     | 0.46              |
| 10:C16:363:PHE:CD2   | 10:C16:367:ASN:ND2   | 2.84                     | 0.46              |
| 10:C16:667:ILE:HA    | 10:C16:670:GLU:N     | 2.31                     | 0.46              |
| 10:C16:729:SER:C     | 10:C16:731:GLN:N     | 2.73                     | 0.46              |
| 10:C16:1496:PHE:CE1  | 10:C16:1498:GLY:O    | 2.69                     | 0.46              |
| 10:C24:1488:ILE:CG2  | 10:C24:1525:VAL:HG13 | 2.45                     | 0.46              |
| 10:C24:1654:LEU:HD22 | 10:C24:1670:PRO:O    | 2.16                     | 0.46              |
| 11:A40:36:ASN:HD22   | 22:I16:293:LYS:HZ3   | 1.61                     | 0.46              |
| 10:C:68:LEU:HB3      | 10:C:69:PRO:HD2      | 1.98                     | 0.46              |
| 10:C:123:TRP:CZ2     | 10:C:127:ARG:HD2     | 2.50                     | 0.46              |
| 10:C:154:ASP:OD1     | 24:D:1403:LEU:CD2    | 2.64                     | 0.46              |
| 10:C:664:ASN:O       | 10:C:668:ALA:N       | 2.42                     | 0.46              |
| 10:C:729:SER:C       | 10:C:731:GLN:H       | 2.24                     | 0.46              |
| 10:C:795:ASP:OD1     | 10:C:796:LEU:N       | 2.49                     | 0.46              |
| 10:C:1002:LEU:HD11   | 10:C:1016:LEU:CD2    | 2.45                     | 0.46              |
| 10:C:1654:LEU:HD22   | 10:C:1670:PRO:O      | 2.16                     | 0.46              |
| 10:C8:62:ILE:HD13    | 10:C8:95:VAL:HG21    | 1.97                     | 0.46              |
| 10:C8:573:GLU:N      | 10:C8:574:PRO:HD2    | 2.30                     | 0.46              |
| 10:C8:768:ARG:HH22   | 10:C8:775:LYS:HG2    | 1.68                     | 0.46              |
| 10:C8:803:ARG:HH21   | 10:C8:808:PRO:CG     | 2.29                     | 0.46              |
| 10:C8:1017:HIS:CD2   | 10:C8:1139:ARG:HD3   | 2.50                     | 0.46              |
| 11:A16:322:ARG:NH1   | 11:A16:351:PHE:HZ    | 2.11                     | 0.46              |
| 11:A16:823:VAL:O     | 11:A16:830:ILE:CD1   | 2.64                     | 0.46              |
| 11:A32:140:TRP:HB2   | 18:B8:1832:LYS:NZ    | 2.30                     | 0.46              |
| 18:B:863:MET:CE      | 18:B:900:LEU:HD21    | 2.46                     | 0.46              |
| 18:B:904:ALA:HB2     | 18:B:917:PHE:CZ      | 2.49                     | 0.46              |
| 18:B:1769:ASN:HA     | 18:B:1812:GLN:OE1    | 2.15                     | 0.46              |
| 18:B8:618:VAL:HG11   | 18:B8:621:VAL:HG21   | 1.97                     | 0.46              |
| 22:I:161:VAL:CG2     | 23:J32:585:LEU:HD21  | 2.46                     | 0.46              |
| 21:H8:363:MET:O      | 21:H8:367:VAL:HG23   | 2.15                     | 0.46              |
| 22:I16:131:ARG:CG    | 23:J16:557:ARG:CZ    | 2.64                     | 0.46              |
| 24:D:1:MET:CG        | 24:D:882:GLU:OE2     | 2.63                     | 0.46              |
| 24:D:308:ASN:CB      | 24:D16:753:ARG:HH21  | 2.29                     | 0.46              |
| 24:D8:1298:ILE:HG22  | 24:D8:1298:ILE:O     | 2.16                     | 0.46              |
| 24:D32:274:MET:HE3   | 24:D32:321:SER:CB    | 2.42                     | 0.46              |
| 24:D40:1298:ILE:HG22 | 24:D40:1298:ILE:O    | 2.16                     | 0.46              |
| 10:C32:573:GLU:N     | 10:C32:574:PRO:HD2   | 2.30                     | 0.46              |
| 10:C32:931:PRO:O     | 10:C32:939:LYS:HD2   | 2.16                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1002:LEU:HD11 | 10:C32:1016:LEU:CD2  | 2.45                     | 0.46              |
| 10:C32:1708:ARG:CB   | 10:C32:1730:ILE:CD1  | 2.93                     | 0.46              |
| 12:A48:820:LEU:HD22  | 12:A48:830:ILE:HG23  | 1.96                     | 0.46              |
| 1:R8:1340:LEU:HD13   | 1:R8:1354:VAL:HG21   | 1.96                     | 0.46              |
| 2:M8:578:ARG:HG2     | 2:M8:587:PHE:HZ      | 1.81                     | 0.46              |
| 2:M16:627:TYR:CE2    | 3:N16:165:GLY:C      | 2.94                     | 0.46              |
| 2:M16:762:LEU:CD1    | 2:M16:813:ASN:ND2    | 2.77                     | 0.46              |
| 2:M16:847:PHE:CD1    | 4:T16:656:TRP:CE3    | 2.59                     | 0.46              |
| 6:O:54:VAL:CG1       | 6:O:85:TRP:NE1       | 2.67                     | 0.46              |
| 5:P8:220:GLU:OE2     | 5:P8:232:ARG:NH2     | 2.49                     | 0.46              |
| 5:P8:483:LEU:HD21    | 5:P8:493:LEU:HD23    | 1.98                     | 0.46              |
| 5:P8:503:VAL:HG11    | 5:P8:528:LEU:HD22    | 1.98                     | 0.46              |
| 8:L8:605:MET:HE2     | 8:L8:634:HIS:CD2     | 2.44                     | 0.46              |
| 9:K:700:MET:HE1      | 9:K:767:LEU:HD13     | 1.96                     | 0.46              |
| 9:K8:743:ARG:NH2     | 9:K8:772:TYR:CE1     | 2.82                     | 0.46              |
| 9:K16:1214:TYR:CE2   | 9:K16:1232:LEU:HD21  | 2.50                     | 0.46              |
| 10:C16:62:ILE:HD13   | 10:C16:95:VAL:HG21   | 1.97                     | 0.46              |
| 10:C16:168:ARG:HH12  | 10:C16:228:ARG:C     | 2.23                     | 0.46              |
| 10:C16:450:PRO:C     | 10:C16:452:LEU:N     | 2.69                     | 0.46              |
| 10:C16:993:HIS:HA    | 10:C16:996:THR:OG1   | 2.16                     | 0.46              |
| 10:C16:1499:ASN:OD1  | 10:C24:1661:LEU:CB   | 2.60                     | 0.46              |
| 11:A24:823:VAL:O     | 11:A24:830:ILE:CD1   | 2.64                     | 0.46              |
| 10:C24:172:ILE:HG23  | 10:C24:240:ILE:CD1   | 2.46                     | 0.46              |
| 10:C24:667:ILE:HA    | 10:C24:670:GLU:N     | 2.31                     | 0.46              |
| 10:C24:1017:HIS:CD2  | 10:C24:1139:ARG:HD3  | 2.50                     | 0.46              |
| 10:C24:1713:ALA:O    | 10:C24:1717:ILE:HG13 | 2.16                     | 0.46              |
| 11:A40:465:SER:C     | 11:A40:467:SER:N     | 2.72                     | 0.46              |
| 15:J:682:ALA:C       | 15:J:684:ASP:H       | 2.23                     | 0.46              |
| 10:C:281:ASP:HB3     | 24:D:1398:ARG:HG3    | 1.95                     | 0.46              |
| 10:C:561:ASN:HA      | 10:C:562:PRO:HD3     | 1.70                     | 0.46              |
| 10:C8:319:ALA:HA     | 10:C8:392:LEU:HD11   | 1.97                     | 0.46              |
| 10:C8:795:ASP:OD1    | 10:C8:796:LEU:N      | 2.49                     | 0.46              |
| 10:C8:1188:TRP:CZ2   | 10:C8:1192:ARG:HD2   | 2.51                     | 0.46              |
| 11:A16:91:GLU:CG     | 18:B:1112:LYS:HD3    | 2.45                     | 0.46              |
| 11:A16:354:ARG:HA    | 11:A16:452:TRP:CE2   | 2.50                     | 0.46              |
| 11:A32:15:HIS:HE1    | 22:I24:165:GLY:O     | 1.96                     | 0.46              |
| 11:A32:388:VAL:CG1   | 11:A32:392:SER:HB2   | 2.46                     | 0.46              |
| 11:A32:676:TYR:OH    | 24:D32:1394:SER:O    | 2.28                     | 0.46              |
| 18:B:32:LEU:HD23     | 18:B:36:ILE:CG2      | 2.46                     | 0.46              |
| 18:B:685:SER:O       | 18:B:687:SER:N       | 2.48                     | 0.46              |
| 18:B:1398:LYS:HE3    | 18:B:1450:ILE:HD11   | 1.98                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:7:VAL:HG12     | 18:B8:8:ASP:N        | 2.31                     | 0.46              |
| 18:B8:1133:THR:C     | 18:B8:1135:ASP:N     | 2.72                     | 0.46              |
| 18:B8:1161:LEU:HG    | 18:B8:1403:ILE:HD13  | 1.96                     | 0.46              |
| 20:E8:274:PRO:HA     | 20:E8:279:GLN:OE1    | 2.15                     | 0.46              |
| 22:I:203:GLN:CD      | 22:I:209:TRP:HZ2     | 2.20                     | 0.46              |
| 22:I24:171:MET:HE1   | 23:J24:595:THR:OG1   | 2.16                     | 0.46              |
| 22:I16:332:MET:CG    | 23:J16:732:MET:HE1   | 2.46                     | 0.46              |
| 24:D8:387:LEU:HD21   | 24:D8:411:MET:HG2    | 1.98                     | 0.46              |
| 24:D8:857:THR:HG21   | 24:D8:885:TYR:CZ     | 2.46                     | 0.46              |
| 24:D16:1298:ILE:HG22 | 24:D16:1298:ILE:O    | 2.16                     | 0.46              |
| 24:D32:552:VAL:HG21  | 24:D32:592:ILE:HD11  | 1.98                     | 0.46              |
| 24:D40:387:LEU:HD21  | 24:D40:411:MET:HG2   | 1.98                     | 0.46              |
| 10:C32:89:LEU:HD11   | 10:C32:123:TRP:HE1   | 1.79                     | 0.46              |
| 10:C32:390:HIS:ND1   | 10:C32:452:LEU:HD22  | 2.30                     | 0.46              |
| 2:M:757:VAL:CG1      | 2:M:758:GLU:N        | 2.79                     | 0.46              |
| 2:M8:250:LEU:HD23    | 2:M8:287:TYR:CZ      | 2.51                     | 0.46              |
| 3:N8:202:CYS:O       | 3:N8:204:PRO:O       | 2.33                     | 0.46              |
| 5:P:139:SER:O        | 5:P:142:SER:OG       | 2.34                     | 0.46              |
| 5:P:503:VAL:HG11     | 5:P:528:LEU:HD22     | 1.98                     | 0.46              |
| 7:Q:341:GLN:CB       | 10:C8:751:ARG:HH11   | 2.28                     | 0.46              |
| 5:P8:62:ASP:OD1      | 5:P8:62:ASP:N        | 2.49                     | 0.46              |
| 5:P8:641:GLN:HE22    | 5:P8:681:ALA:CB      | 2.29                     | 0.46              |
| 5:P16:47:ASN:CG      | 5:P16:471:SER:HG     | 2.12                     | 0.46              |
| 9:K:601:VAL:CG1      | 9:K:673:SER:HB3      | 2.38                     | 0.46              |
| 9:K:839:LEU:O        | 9:K:842:ILE:HG22     | 2.16                     | 0.46              |
| 9:K8:1019:ARG:HD3    | 9:K8:1059:ARG:HD2    | 1.97                     | 0.46              |
| 10:C16:837:ARG:NH2   | 10:C16:890:ASP:O     | 2.49                     | 0.46              |
| 10:C16:931:PRO:O     | 10:C16:939:LYS:HD2   | 2.16                     | 0.46              |
| 10:C16:1017:HIS:CD2  | 10:C16:1139:ARG:HD3  | 2.50                     | 0.46              |
| 10:C16:1215:ALA:O    | 10:C16:1219:ILE:HB   | 2.16                     | 0.46              |
| 10:C16:1713:ALA:O    | 10:C16:1717:ILE:HG13 | 2.16                     | 0.46              |
| 11:A24:72:ILE:HD13   | 21:H8:348:ALA:CB     | 2.46                     | 0.46              |
| 10:C24:68:LEU:HB3    | 10:C24:69:PRO:HD2    | 1.98                     | 0.46              |
| 10:C24:1102:SER:C    | 10:C24:1104:GLN:H    | 2.24                     | 0.46              |
| 11:A40:468:VAL:HG11  | 24:D32:1100:GLN:HB3  | 1.96                     | 0.46              |
| 11:A40:526:GLY:C     | 11:A40:528:GLY:H     | 2.23                     | 0.46              |
| 11:A40:823:VAL:O     | 11:A40:830:ILE:CD1   | 2.64                     | 0.46              |
| 12:A:144:LYS:CE      | 10:C:1821:VAL:CG1    | 2.93                     | 0.46              |
| 12:A:322:ARG:NH1     | 12:A:351:PHE:HZ      | 2.11                     | 0.46              |
| 13:V:744:LEU:O       | 13:V:747:SER:OG      | 2.27                     | 0.46              |
| 14:W:711:ARG:HH11    | 10:C8:1609:ASP:HB2   | 0.68                     | 0.46              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C:225:LEU:HD21    | 10:C:388:TYR:CE2    | 2.51                     | 0.46              |
| 10:C:605:GLU:H       | 10:C:605:GLU:HG2    | 1.47                     | 0.46              |
| 10:C:993:HIS:HA      | 10:C:996:THR:OG1    | 2.16                     | 0.46              |
| 10:C8:172:ILE:HG23   | 10:C8:240:ILE:CD1   | 2.46                     | 0.46              |
| 10:C8:931:PRO:O      | 10:C8:939:LYS:HD2   | 2.16                     | 0.46              |
| 11:A32:90:PHE:CG     | 18:B8:1788:ILE:CD1  | 2.85                     | 0.46              |
| 11:A32:124:ASN:CB    | 18:B8:1523:ARG:NH1  | 2.78                     | 0.46              |
| 11:A32:782:PRO:C     | 11:A32:783:PHE:CG   | 2.93                     | 0.46              |
| 18:B:171:ILE:CD1     | 18:B:226:TYR:HB3    | 2.36                     | 0.46              |
| 18:B:268:GLN:HE22    | 18:B:323:GLU:CG     | 2.29                     | 0.46              |
| 18:B8:652:LEU:HD21   | 18:B8:724:LEU:HD23  | 1.97                     | 0.46              |
| 20:E:24:ILE:HB       | 20:E:25:PRO:CD      | 2.45                     | 0.46              |
| 22:I8:171:MET:HE1    | 23:J8:595:THR:OG1   | 2.16                     | 0.46              |
| 24:D:403:ARG:NH2     | 24:D16:748:GLU:HB2  | 2.31                     | 0.46              |
| 24:D:1298:ILE:HG22   | 24:D:1298:ILE:O     | 2.16                     | 0.46              |
| 24:D16:1109:LEU:CD2  | 24:D16:1156:SER:HB2 | 2.45                     | 0.46              |
| 24:D24:1298:ILE:HG22 | 24:D24:1298:ILE:O   | 2.16                     | 0.46              |
| 10:C32:1033:GLY:C    | 10:C32:1218:ARG:NH2 | 2.70                     | 0.46              |
| 10:C32:1215:ALA:O    | 10:C32:1219:ILE:HB  | 2.16                     | 0.46              |
| 10:C32:1424:GLN:HE22 | 10:C32:1478:VAL:CG1 | 2.26                     | 0.46              |
| 1:R:93:SER:HB2       | 1:R:685:ILE:HD12    | 1.98                     | 0.46              |
| 3:N:227:SER:HB2      | 3:N:243:VAL:HG12    | 1.98                     | 0.46              |
| 1:R16:1139:ARG:HG3   | 1:R16:1157:ARG:CZ   | 2.45                     | 0.46              |
| 2:M16:211:MET:HE3    | 3:N16:280:ASN:CA    | 2.46                     | 0.46              |
| 2:M16:578:ARG:HG2    | 2:M16:587:PHE:HZ    | 1.81                     | 0.46              |
| 2:M16:625:HIS:HE2    | 3:N16:225:PRO:CA    | 2.26                     | 0.46              |
| 5:P:475:THR:O        | 5:P:478:ILE:HG12    | 2.16                     | 0.46              |
| 5:P16:43:TRP:HH2     | 5:P16:76:LEU:HD12   | 1.81                     | 0.46              |
| 5:P16:62:ASP:N       | 5:P16:62:ASP:OD1    | 2.49                     | 0.46              |
| 5:P16:256:HIS:HE1    | 5:P16:270:GLU:OE1   | 1.99                     | 0.46              |
| 8:L8:608:PHE:CE2     | 8:L8:635:MET:CG     | 2.98                     | 0.46              |
| 8:L8:613:GLU:OE1     | 8:L8:639:ARG:NE     | 2.49                     | 0.46              |
| 8:L16:601:HIS:HE1    | 8:L16:631:LEU:HB2   | 1.81                     | 0.46              |
| 9:K:798:LEU:HB3      | 9:K:842:ILE:HD11    | 1.97                     | 0.46              |
| 9:K:938:PHE:HD1      | 9:K:965:LEU:HD11    | 1.81                     | 0.46              |
| 9:K8:839:LEU:O       | 9:K8:842:ILE:HG22   | 2.16                     | 0.46              |
| 9:K8:847:LEU:HD22    | 9:K8:910:SER:CB     | 2.43                     | 0.46              |
| 9:K8:894:LYS:CD      | 9:K8:1058:GLU:HG2   | 2.24                     | 0.46              |
| 9:K8:1034:PHE:HB2    | 9:K8:1088:ASP:HB2   | 1.98                     | 0.46              |
| 9:K8:1113:ILE:HD12   | 9:K8:1132:LEU:CD2   | 2.45                     | 0.46              |
| 10:C16:573:GLU:OE1   | 10:C16:617:TYR:OH   | 2.32                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A24:526:GLY:C    | 11:A24:528:GLY:H    | 2.23                     | 0.46              |
| 11:A24:587:VAL:HG22 | 11:A24:627:ILE:CD1  | 2.46                     | 0.46              |
| 10:C24:62:ILE:HD13  | 10:C24:95:VAL:HG21  | 1.97                     | 0.46              |
| 10:C24:1215:ALA:O   | 10:C24:1219:ILE:HB  | 2.16                     | 0.46              |
| 10:C24:1496:PHE:CE1 | 10:C24:1498:GLY:O   | 2.69                     | 0.46              |
| 10:C24:1757:GLN:OE1 | 11:A40:136:LEU:HD23 | 2.11                     | 0.46              |
| 11:A40:749:GLN:NE2  | 24:D24:1398:ARG:CD  | 2.79                     | 0.46              |
| 13:V:902:MET:HG2    | 15:J:696:LEU:HD21   | 1.95                     | 0.46              |
| 15:J:689:LEU:O      | 15:J:693:VAL:HG23   | 2.16                     | 0.46              |
| 10:C:1708:ARG:CG    | 10:C:1730:ILE:CD1   | 2.94                     | 0.46              |
| 10:C8:265:PHE:CE1   | 10:C8:389:LEU:HD12  | 2.50                     | 0.46              |
| 11:A16:20:LEU:CD1   | 21:H:346:THR:CG2    | 2.90                     | 0.46              |
| 11:A32:440:LEU:O    | 11:A32:443:LEU:HD12 | 2.16                     | 0.46              |
| 11:A32:823:VAL:O    | 11:A32:830:ILE:CD1  | 2.64                     | 0.46              |
| 18:B:274:ILE:O      | 18:B:278:THR:HG23   | 2.16                     | 0.46              |
| 18:B:729:LEU:CG     | 18:B:1196:MET:HE1   | 2.45                     | 0.46              |
| 18:B:1209:LEU:CD2   | 18:B:1238:PHE:HE1   | 2.29                     | 0.46              |
| 18:B8:274:ILE:O     | 18:B8:278:THR:HG23  | 2.16                     | 0.46              |
| 18:B8:530:SER:O     | 18:B8:531:ASN:HB2   | 2.16                     | 0.46              |
| 18:B8:537:LEU:HD11  | 18:B8:548:ARG:HB2   | 1.97                     | 0.46              |
| 18:B8:688:GLY:O     | 18:B8:690:TRP:N     | 2.49                     | 0.46              |
| 18:B8:729:LEU:CG    | 18:B8:1196:MET:HE1  | 2.45                     | 0.46              |
| 18:B8:1275:TYR:OH   | 18:B8:1300:GLU:OE2  | 2.25                     | 0.46              |
| 18:B8:1398:LYS:HE3  | 18:B8:1450:ILE:HD11 | 1.98                     | 0.46              |
| 21:H:363:MET:O      | 21:H:367:VAL:HG23   | 2.15                     | 0.46              |
| 21:H8:284:LEU:CD2   | 23:J8:647:MET:O     | 2.64                     | 0.46              |
| 21:H24:217:ARG:HH21 | 23:J24:586:GLU:CD   | 2.23                     | 0.46              |
| 22:I16:303:SER:O    | 22:I16:307:VAL:HG23 | 2.16                     | 0.46              |
| 24:D:552:VAL:HG21   | 24:D:592:ILE:HD11   | 1.97                     | 0.46              |
| 10:C32:54:ARG:HE    | 10:C32:81:LEU:HD22  | 1.80                     | 0.46              |
| 10:C32:450:PRO:C    | 10:C32:452:LEU:N    | 2.69                     | 0.46              |
| 12:A48:629:LEU:HD22 | 12:A48:675:LEU:CD1  | 2.46                     | 0.46              |
| 1:R:1335:ILE:HG13   | 10:C:1170:VAL:HG22  | 1.92                     | 0.46              |
| 1:R:1379:GLN:O      | 1:R:1380:LYS:C      | 2.56                     | 0.46              |
| 2:M:851:LEU:CD2     | 4:T:653:GLN:CG      | 2.85                     | 0.46              |
| 3:N:9:GLY:C         | 3:N:36:LYS:NZ       | 2.74                     | 0.46              |
| 1:R8:765:ASP:OD1    | 24:D40:1361:ALA:O   | 2.32                     | 0.46              |
| 1:R8:983:ARG:NH2    | 24:D40:1366:PRO:HD3 | 2.30                     | 0.46              |
| 1:R16:93:SER:HB2    | 1:R16:685:ILE:HD12  | 1.98                     | 0.46              |
| 3:N16:9:GLY:C       | 3:N16:36:LYS:NZ     | 2.74                     | 0.46              |
| 7:Q:51:ILE:HG12     | 7:Q:121:ILE:HD11    | 1.98                     | 0.46              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P8:105:ARG:CZ      | 5:P8:130:VAL:CA     | 2.83                     | 0.46              |
| 9:K8:1279:GLU:O      | 9:K8:1281:SER:N     | 2.49                     | 0.46              |
| 10:C16:1002:LEU:HD11 | 10:C16:1016:LEU:CD2 | 2.45                     | 0.46              |
| 10:C16:1062:GLU:HA   | 10:C16:1063:PRO:HD3 | 1.68                     | 0.46              |
| 10:C16:1663:SER:C    | 10:C24:1564:ASP:OD2 | 2.54                     | 0.46              |
| 11:A24:107:GLN:CD    | 21:H8:325:PRO:HA    | 2.40                     | 0.46              |
| 10:C24:398:SER:HA    | 10:C24:458:VAL:CG1  | 2.46                     | 0.46              |
| 10:C24:1050:HIS:CD2  | 10:C24:1086:LYS:HZ1 | 1.96                     | 0.46              |
| 10:C24:1283:LEU:CD2  | 10:C24:1287:MET:HE2 | 2.45                     | 0.46              |
| 12:A:526:GLY:C       | 12:A:528:GLY:H      | 2.23                     | 0.46              |
| 13:V:835:GLU:CB      | 15:J:648:TYR:OH     | 2.64                     | 0.46              |
| 10:C:54:ARG:HE       | 10:C:81:LEU:HD22    | 1.80                     | 0.46              |
| 10:C8:1102:SER:C     | 10:C8:1104:GLN:H    | 2.24                     | 0.46              |
| 10:C8:1271:PHE:CD1   | 10:C8:1731:HIS:NE2  | 2.75                     | 0.46              |
| 10:C8:1352:GLN:HE22  | 10:C8:1357:LEU:CD1  | 2.29                     | 0.46              |
| 11:A32:90:PHE:CB     | 18:B8:1788:ILE:CD1  | 2.17                     | 0.46              |
| 18:B:147:LYS:NZ      | 18:B:384:ASP:O      | 2.49                     | 0.46              |
| 18:B:624:ILE:O       | 18:B:627:SER:OG     | 2.19                     | 0.46              |
| 18:B:712:PRO:HB2     | 18:B:759:MET:CE     | 2.43                     | 0.46              |
| 18:B:1215:PHE:HZ     | 18:B:1234:MET:SD    | 2.34                     | 0.46              |
| 18:B:1575:GLN:HG2    | 24:D16:1403:LEU:HB3 | 1.98                     | 0.46              |
| 18:B:1804:THR:O      | 18:B:1805:GLU:C     | 2.55                     | 0.46              |
| 18:B8:268:GLN:HE22   | 18:B8:323:GLU:CG    | 2.29                     | 0.46              |
| 18:B8:374:ILE:CG2    | 18:B8:380:LEU:HD13  | 2.46                     | 0.46              |
| 18:B8:973:ASP:O      | 18:B8:974:SER:C     | 2.52                     | 0.46              |
| 18:B8:1098:MET:HE1   | 18:B8:1142:PHE:CB   | 2.46                     | 0.46              |
| 18:B8:1677:ARG:O     | 18:B8:1679:ARG:N    | 2.49                     | 0.46              |
| 18:B8:1947:GLU:N     | 18:B8:1948:PRO:CD   | 2.79                     | 0.46              |
| 20:E:355:PRO:O       | 20:E:454:MET:HE1    | 2.16                     | 0.46              |
| 19:48:23:GLN:O       | 19:48:24:ASN:OD1    | 2.33                     | 0.46              |
| 20:E8:353:ILE:HG21   | 20:E8:413:PHE:HE2   | 1.29                     | 0.46              |
| 21:H8:271:LEU:HD21   | 22:I8:254:ILE:HG21  | 1.98                     | 0.46              |
| 22:I8:155:PHE:CZ     | 22:I8:159:ARG:HD2   | 2.51                     | 0.46              |
| 22:I8:161:VAL:CG2    | 23:J8:585:LEU:HD21  | 2.46                     | 0.46              |
| 21:H16:208:ASP:OD2   | 22:I16:142:ARG:NH2  | 2.50                     | 0.46              |
| 21:H16:217:ARG:HH21  | 23:J16:586:GLU:CD   | 2.23                     | 0.46              |
| 22:I16:171:MET:HE1   | 23:J16:595:THR:OG1  | 2.16                     | 0.46              |
| 24:D24:853:MET:CB    | 24:D24:885:TYR:CD2  | 2.93                     | 0.46              |
| 10:C32:168:ARG:HH22  | 10:C32:227:ASP:C    | 2.23                     | 0.46              |
| 10:C32:265:PHE:CE1   | 10:C32:389:LEU:HD12 | 2.50                     | 0.46              |
| 10:C32:460:TRP:CZ2   | 10:C32:495:LYS:HD2  | 2.51                     | 0.46              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C32:1188:TRP:CZ2 | 10:C32:1192:ARG:HD2  | 2.51                     | 0.46              |
| 10:C32:1496:PHE:CE1 | 10:C32:1498:GLY:O    | 2.69                     | 0.46              |
| 10:C32:1713:ALA:O   | 10:C32:1717:ILE:HG13 | 2.16                     | 0.46              |
| 1:R:1033:LYS:HE2    | 24:D:1436:ARG:NE     | 2.31                     | 0.45              |
| 2:M:622:ARG:CZ      | 2:M:624:ASP:OD2      | 2.64                     | 0.45              |
| 2:M:673:ASN:OD1     | 2:M:681:ALA:HB2      | 2.16                     | 0.45              |
| 2:M16:420:CYS:HB3   | 8:L16:391:TRP:HZ3    | 1.71                     | 0.45              |
| 2:M16:562:PHE:CE2   | 3:N16:295:GLU:CD     | 2.95                     | 0.45              |
| 6:O:5:MET:CE        | 6:O:46:PHE:CE2       | 2.99                     | 0.45              |
| 5:P8:39:LEU:HD11    | 6:O8:323:PRO:HG2     | 1.98                     | 0.45              |
| 6:O16:173:VAL:HG22  | 6:O16:189:LEU:HD12   | 1.92                     | 0.45              |
| 7:Q16:297:VAL:HG13  | 7:Q16:301:ARG:CB     | 2.44                     | 0.45              |
| 8:L8:605:MET:CE     | 8:L8:634:HIS:HD2     | 2.28                     | 0.45              |
| 9:K8:938:PHE:HD1    | 9:K8:965:LEU:HD11    | 1.81                     | 0.45              |
| 9:K8:1113:ILE:HD13  | 9:K8:1136:CYS:SG     | 2.55                     | 0.45              |
| 9:K8:1164:ARG:NH2   | 9:K8:1242:SER:O      | 2.49                     | 0.45              |
| 9:K16:707:GLN:NE2   | 9:K16:734:TRP:CE3    | 2.84                     | 0.45              |
| 10:C16:717:GLU:HG3  | 23:J8:656:ARG:CZ     | 2.45                     | 0.45              |
| 10:C16:1601:TYR:C   | 10:C24:1665:THR:CG2  | 2.88                     | 0.45              |
| 10:C16:1616:ILE:O   | 10:C16:1618:SER:N    | 2.46                     | 0.45              |
| 11:A24:156:MET:HG2  | 11:A24:555:HIS:NE2   | 1.53                     | 0.45              |
| 11:A24:440:LEU:O    | 11:A24:443:LEU:HD12  | 2.16                     | 0.45              |
| 11:A24:465:SER:C    | 11:A24:467:SER:N     | 2.72                     | 0.45              |
| 10:C24:390:HIS:HD1  | 10:C24:452:LEU:HB3   | 1.80                     | 0.45              |
| 10:C24:795:ASP:OD1  | 10:C24:796:LEU:N     | 2.49                     | 0.45              |
| 10:C24:1188:TRP:CZ2 | 10:C24:1192:ARG:HD2  | 2.51                     | 0.45              |
| 10:C24:1728:ASP:N   | 21:H24:275:LYS:HE3   | 2.31                     | 0.45              |
| 11:A40:440:LEU:O    | 11:A40:443:LEU:HD12  | 2.16                     | 0.45              |
| 11:A40:587:VAL:HG22 | 11:A40:627:ILE:CD1   | 2.46                     | 0.45              |
| 12:A:587:VAL:HG22   | 12:A:627:ILE:CD1     | 2.46                     | 0.45              |
| 10:C:18:THR:CG2     | 10:C:883:GLU:CG      | 2.74                     | 0.45              |
| 10:C:168:ARG:HH22   | 10:C:227:ASP:C       | 2.23                     | 0.45              |
| 10:C:1102:SER:C     | 10:C:1104:GLN:H      | 2.24                     | 0.45              |
| 10:C8:363:PHE:CD2   | 10:C8:367:ASN:ND2    | 2.84                     | 0.45              |
| 10:C8:993:HIS:HA    | 10:C8:996:THR:OG1    | 2.16                     | 0.45              |
| 10:C8:1164:VAL:HG13 | 10:C8:1167:PHE:HE2   | 1.81                     | 0.45              |
| 18:B:132:LEU:HD11   | 18:B:199:LEU:HD11    | 1.88                     | 0.45              |
| 18:B:1677:ARG:O     | 18:B:1679:ARG:N      | 2.49                     | 0.45              |
| 18:B8:147:LYS:NZ    | 18:B8:384:ASP:O      | 2.49                     | 0.45              |
| 18:B8:603:PHE:HB3   | 18:B8:619:ARG:CZ     | 2.40                     | 0.45              |
| 18:B8:712:PRO:HB2   | 18:B8:759:MET:CE     | 2.43                     | 0.45              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 21:H:208:ASP:OD2     | 22:I:142:ARG:NH2    | 2.50                     | 0.45              |
| 21:H:275:LYS:HG3     | 21:H:276:GLY:N      | 2.30                     | 0.45              |
| 21:H:284:LEU:CD2     | 23:J32:647:MET:O    | 2.64                     | 0.45              |
| 22:I:303:SER:O       | 22:I:307:VAL:HG23   | 2.16                     | 0.45              |
| 24:D8:274:MET:HE3    | 24:D8:321:SER:CB    | 2.42                     | 0.45              |
| 24:D24:552:VAL:HG21  | 24:D24:592:ILE:HD11 | 1.97                     | 0.45              |
| 10:C32:229:PRO:HG2   | 10:C32:270:THR:CG2  | 2.45                     | 0.45              |
| 10:C32:1654:LEU:HD22 | 10:C32:1670:PRO:O   | 2.16                     | 0.45              |
| 12:A48:587:VAL:HG22  | 12:A48:627:ILE:CD1  | 2.46                     | 0.45              |
| 1:R:1124:TRP:HH2     | 4:T:669:PRO:CA      | 2.28                     | 0.45              |
| 1:R:1422:SER:HB2     | 6:O:132:TYR:CE2     | 2.51                     | 0.45              |
| 2:M:578:ARG:HG2      | 2:M:587:PHE:HZ      | 1.81                     | 0.45              |
| 3:N:222:LEU:CD1      | 3:N:270:THR:HA      | 2.44                     | 0.45              |
| 1:R8:768:LEU:HA      | 1:R8:768:LEU:HD13   | 1.78                     | 0.45              |
| 2:M8:730:GLU:HG3     | 8:L16:504:GLN:CD    | 2.36                     | 0.45              |
| 3:N16:227:SER:HB2    | 3:N16:243:VAL:HG12  | 1.98                     | 0.45              |
| 7:Q:183:ARG:HD3      | 7:Q:229:ILE:CG2     | 2.46                     | 0.45              |
| 5:P8:112:LEU:HD13    | 5:P8:123:GLN:HE21   | 1.75                     | 0.45              |
| 5:P8:256:HIS:HE1     | 5:P8:270:GLU:OE1    | 1.98                     | 0.45              |
| 7:Q16:290:ASP:OD2    | 7:Q16:293:THR:OG1   | 2.27                     | 0.45              |
| 10:C16:172:ILE:HG23  | 10:C16:240:ILE:CD1  | 2.46                     | 0.45              |
| 10:C16:795:ASP:OD1   | 10:C16:796:LEU:N    | 2.49                     | 0.45              |
| 10:C16:1699:LYS:CE   | 23:J32:722:LEU:CD2  | 2.92                     | 0.45              |
| 11:A24:359:GLU:OE2   | 11:A24:362:ARG:NH2  | 2.50                     | 0.45              |
| 11:A24:388:VAL:CG1   | 11:A24:392:SER:HB2  | 2.46                     | 0.45              |
| 10:C24:553:LEU:HD23  | 10:C24:595:THR:CG2  | 2.44                     | 0.45              |
| 10:C24:837:ARG:NH2   | 10:C24:890:ASP:O    | 2.49                     | 0.45              |
| 10:C24:1626:GLN:NE2  | 10:C24:1692:LYS:HZ3 | 1.99                     | 0.45              |
| 10:C24:1821:VAL:CG1  | 11:A40:144:LYS:CE   | 2.93                     | 0.45              |
| 12:A:132:MET:CE      | 10:C:1530:PHE:CE1   | 2.92                     | 0.45              |
| 13:V:839:LYS:NZ      | 15:J:652:GLU:CG     | 2.72                     | 0.45              |
| 13:V:906:LEU:HD12    | 14:W:784:LEU:HD12   | 1.98                     | 0.45              |
| 14:W:585:ILE:CG2     | 15:J:572:ASP:HB3    | 2.46                     | 0.45              |
| 10:C:35:ASN:CG       | 24:D:1148:LEU:CD1   | 2.80                     | 0.45              |
| 10:C:172:ILE:HG23    | 10:C:240:ILE:CD1    | 2.46                     | 0.45              |
| 10:C:573:GLU:N       | 10:C:574:PRO:HD2    | 2.30                     | 0.45              |
| 10:C8:168:ARG:HH12   | 10:C8:228:ARG:C     | 2.23                     | 0.45              |
| 10:C8:909:PRO:CB     | 10:C8:920:LEU:HD22  | 2.46                     | 0.45              |
| 10:C8:1389:ILE:HD12  | 10:C8:1426:ARG:NH1  | 2.23                     | 0.45              |
| 10:C8:1537:GLU:OE2   | 10:C8:1540:GLU:CD   | 2.59                     | 0.45              |
| 11:A16:388:VAL:CG1   | 11:A16:392:SER:HB2  | 2.45                     | 0.45              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A16:587:VAL:HG22  | 11:A16:627:ILE:CD1  | 2.46                     | 0.45              |
| 11:A16:629:LEU:HD22  | 11:A16:675:LEU:CD1  | 2.46                     | 0.45              |
| 11:A32:629:LEU:HD22  | 11:A32:675:LEU:CD1  | 2.46                     | 0.45              |
| 18:B:460:PRO:CB      | 18:B:562:ARG:NH1    | 2.76                     | 0.45              |
| 18:B:460:PRO:CB      | 18:B:562:ARG:HH11   | 2.26                     | 0.45              |
| 18:B:467:ILE:HG23    | 18:B:581:LEU:HD22   | 1.98                     | 0.45              |
| 18:B:537:LEU:HD11    | 18:B:548:ARG:HB2    | 1.97                     | 0.45              |
| 18:B:1068:THR:C      | 18:B:1070:GLY:N     | 2.74                     | 0.45              |
| 18:B:1419:LYS:CG     | 18:B:1468:PHE:HE1   | 2.17                     | 0.45              |
| 18:B:1652:PHE:HZ     | 18:B:1700:LEU:HD12  | 1.81                     | 0.45              |
| 18:B:1700:LEU:HD21   | 18:B:1833:PHE:CE2   | 2.50                     | 0.45              |
| 18:B:1947:GLU:N      | 18:B:1948:PRO:CD    | 2.79                     | 0.45              |
| 18:B8:32:LEU:HD23    | 18:B8:36:ILE:CG2    | 2.46                     | 0.45              |
| 18:B8:690:TRP:HE3    | 18:B8:739:VAL:CG2   | 1.94                     | 0.45              |
| 18:B8:863:MET:CE     | 18:B8:900:LEU:HD21  | 2.46                     | 0.45              |
| 18:B8:1110:LEU:HD21  | 21:H24:326:GLY:H    | 1.58                     | 0.45              |
| 18:B8:1658:MET:HE3   | 18:B8:1662:TYR:HE2  | 1.81                     | 0.45              |
| 19:4:251:ARG:NH2     | 19:4:254:LEU:CD2    | 2.79                     | 0.45              |
| 20:E:432:ILE:HG22    | 20:E:434:TRP:HD1    | 1.80                     | 0.45              |
| 20:E8:206:GLY:O      | 20:E8:208:VAL:N     | 2.46                     | 0.45              |
| 21:H8:255:LEU:HD21   | 22:I8:265:THR:HG21  | 1.97                     | 0.45              |
| 21:H16:255:LEU:HD21  | 22:I16:265:THR:HG21 | 1.97                     | 0.45              |
| 21:H16:284:LEU:CD2   | 23:J16:647:MET:O    | 2.64                     | 0.45              |
| 24:D:387:LEU:HD21    | 24:D:411:MET:HG2    | 1.98                     | 0.45              |
| 24:D24:274:MET:HE3   | 24:D24:321:SER:CB   | 2.43                     | 0.45              |
| 24:D32:1298:ILE:HG22 | 24:D32:1298:ILE:O   | 2.16                     | 0.45              |
| 10:C32:803:ARG:HH21  | 10:C32:808:PRO:CG   | 2.28                     | 0.45              |
| 10:C32:969:ASN:OD1   | 10:C32:979:MET:HE2  | 2.17                     | 0.45              |
| 12:A48:557:LEU:CD2   | 12:A48:561:ASP:CB   | 2.90                     | 0.45              |
| 1:R:768:LEU:HD11     | 24:D:1313:LEU:HD11  | 1.99                     | 0.45              |
| 3:N:1:MET:O          | 3:N:302:PRO:C       | 2.60                     | 0.45              |
| 2:M8:225:ASP:CB      | 2:M8:606:GLN:HE22   | 2.28                     | 0.45              |
| 5:P:483:LEU:HD21     | 5:P:493:LEU:HD23    | 1.98                     | 0.45              |
| 5:P8:139:SER:O       | 5:P8:142:SER:OG     | 2.34                     | 0.45              |
| 6:O8:54:VAL:CG1      | 6:O8:85:TRP:NE1     | 2.67                     | 0.45              |
| 5:P16:105:ARG:NH2    | 5:P16:133:TYR:CB    | 2.79                     | 0.45              |
| 9:K8:716:ALA:O       | 10:C32:503:THR:HG21 | 2.16                     | 0.45              |
| 9:K8:923:ILE:HG22    | 9:K8:929:ARG:CZ     | 2.46                     | 0.45              |
| 9:K16:751:LEU:HD13   | 9:K16:759:VAL:HG13  | 1.98                     | 0.45              |
| 10:C16:909:PRO:CB    | 10:C16:920:LEU:HD22 | 2.46                     | 0.45              |
| 10:C16:1449:GLU:CD   | 24:D8:1151:SER:CA   | 2.81                     | 0.45              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C16:1601:TYR:O   | 10:C24:1665:THR:HG23 | 2.16                     | 0.45              |
| 11:A24:259:ILE:HG23 | 11:A24:276:LEU:HD22  | 1.96                     | 0.45              |
| 10:C24:54:ARG:HE    | 10:C24:81:LEU:HD22   | 1.80                     | 0.45              |
| 10:C24:909:PRO:CB   | 10:C24:920:LEU:HD22  | 2.46                     | 0.45              |
| 10:C24:969:ASN:OD1  | 10:C24:979:MET:HE2   | 2.17                     | 0.45              |
| 11:A40:20:LEU:CD1   | 21:H16:346:THR:CG2   | 2.90                     | 0.45              |
| 13:V:730:GLN:CB     | 13:V:731:PRO:HD3     | 2.47                     | 0.45              |
| 13:V:905:GLN:NE2    | 15:J:700:LEU:HB2     | 2.31                     | 0.45              |
| 14:W:701:LEU:HD13   | 15:J:624:ALA:HB1     | 1.93                     | 0.45              |
| 10:C:64:LEU:CD1     | 10:C:70:ILE:HD12     | 2.42                     | 0.45              |
| 10:C:729:SER:C      | 10:C:731:GLN:N       | 2.73                     | 0.45              |
| 10:C:969:ASN:OD1    | 10:C:979:MET:HE2     | 2.17                     | 0.45              |
| 10:C:1381:ALA:O     | 10:C:1385:LEU:HB2    | 2.17                     | 0.45              |
| 10:C8:394:SER:HA    | 10:C8:458:VAL:HG11   | 1.98                     | 0.45              |
| 10:C8:460:TRP:CZ2   | 10:C8:495:LYS:HD2    | 2.51                     | 0.45              |
| 10:C8:832:LEU:HG    | 10:C8:834:GLN:OE1    | 2.17                     | 0.45              |
| 11:A16:124:ASN:CB   | 18:B:1523:ARG:NH1    | 2.79                     | 0.45              |
| 11:A16:154:ILE:CG2  | 18:B:1851:VAL:CG2    | 2.94                     | 0.45              |
| 17:F8:72:SER:C      | 17:F8:74:ILE:H       | 2.24                     | 0.45              |
| 18:B:135:TYR:OH     | 18:B:139:ARG:NH1     | 2.47                     | 0.45              |
| 18:B:1119:LYS:C     | 18:B:1120:THR:O      | 2.59                     | 0.45              |
| 18:B:1714:MET:O     | 18:B:1718:ASP:HB2    | 2.15                     | 0.45              |
| 18:B8:140:GLN:NE2   | 18:B8:206:GLU:CD     | 2.62                     | 0.45              |
| 18:B8:245:LEU:HD21  | 18:B8:268:GLN:NE2    | 2.32                     | 0.45              |
| 18:B8:685:SER:O     | 18:B8:687:SER:N      | 2.48                     | 0.45              |
| 18:B8:1068:THR:C    | 18:B8:1070:GLY:N     | 2.74                     | 0.45              |
| 18:B8:1529:GLU:CD   | 24:D32:1415:LEU:CG   | 2.78                     | 0.45              |
| 20:E:440:VAL:C      | 20:E:442:LYS:N       | 2.74                     | 0.45              |
| 24:D:122:GLN:HE22   | 24:D:151:VAL:HG21    | 1.82                     | 0.45              |
| 24:D24:122:GLN:HE22 | 24:D24:151:VAL:HG21  | 1.81                     | 0.45              |
| 10:C32:1708:ARG:CG  | 10:C32:1730:ILE:CD1  | 2.94                     | 0.45              |
| 12:A48:359:GLU:OE2  | 12:A48:362:ARG:NH2   | 2.50                     | 0.45              |
| 1:R8:93:SER:HB2     | 1:R8:685:ILE:HD12    | 1.98                     | 0.45              |
| 1:R8:982:GLU:CG     | 24:D40:1436:ARG:HE   | 2.28                     | 0.45              |
| 2:M8:562:PHE:CE2    | 3:N8:295:GLU:CD      | 2.95                     | 0.45              |
| 2:M8:757:VAL:CG1    | 2:M8:758:GLU:N       | 2.79                     | 0.45              |
| 1:R16:1124:TRP:HH2  | 4:T16:669:PRO:HA     | 1.81                     | 0.45              |
| 2:M16:757:VAL:CG1   | 2:M16:758:GLU:N      | 2.79                     | 0.45              |
| 3:N16:128:ASN:HB3   | 3:N16:144:ARG:HE     | 1.81                     | 0.45              |
| 5:P:36:VAL:HG21     | 6:O:323:PRO:HB2      | 1.99                     | 0.45              |
| 5:P:201:ILE:HD12    | 5:P:211:TYR:CZ       | 2.51                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:O8:288:TRP:CE2     | 6:O8:295:LEU:HD13    | 2.52                     | 0.45              |
| 5:P16:36:VAL:HG21    | 6:O16:323:PRO:HB2    | 1.99                     | 0.45              |
| 5:P16:592:SER:HG     | 5:P16:598:LEU:CD1    | 2.07                     | 0.45              |
| 7:Q16:51:ILE:HG12    | 7:Q16:121:ILE:HD11   | 1.98                     | 0.45              |
| 9:K:909:ASP:OD1      | 9:K:957:ILE:HD11     | 2.17                     | 0.45              |
| 9:K8:876:LEU:HD21    | 9:K8:904:ARG:HG3     | 1.98                     | 0.45              |
| 10:C16:225:LEU:HD21  | 10:C16:388:TYR:CE2   | 2.51                     | 0.45              |
| 10:C16:969:ASN:OD1   | 10:C16:979:MET:HE2   | 2.17                     | 0.45              |
| 10:C16:1424:GLN:HE21 | 10:C16:1478:VAL:HG13 | 1.71                     | 0.45              |
| 11:A24:20:LEU:CD1    | 21:H8:346:THR:CG2    | 2.90                     | 0.45              |
| 11:A24:307:GLY:O     | 20:E:387:LEU:HD23    | 2.16                     | 0.45              |
| 11:A24:696:ILE:HD11  | 11:A24:728:ILE:HD12  | 1.92                     | 0.45              |
| 10:C24:225:LEU:HD21  | 10:C24:388:TYR:CE2   | 2.51                     | 0.45              |
| 10:C24:390:HIS:CD2   | 10:C24:449:GLU:CD    | 2.86                     | 0.45              |
| 10:C24:1161:PHE:O    | 10:C24:1162:PRO:C    | 2.55                     | 0.45              |
| 11:A40:388:VAL:CG1   | 11:A40:392:SER:HB2   | 2.45                     | 0.45              |
| 11:A40:587:VAL:CG2   | 11:A40:627:ILE:HD13  | 2.47                     | 0.45              |
| 11:A40:737:GLU:HG2   | 24:D32:802:PHE:CE2   | 2.52                     | 0.45              |
| 11:A40:748:GLU:CB    | 24:D24:1398:ARG:NH1  | 2.26                     | 0.45              |
| 12:A:587:VAL:CG2     | 12:A:627:ILE:HD13    | 2.47                     | 0.45              |
| 14:W:586:ILE:HD13    | 15:J:569:ALA:CA      | 2.22                     | 0.45              |
| 10:C:363:PHE:CD2     | 10:C:367:ASN:ND2     | 2.84                     | 0.45              |
| 10:C:450:PRO:C       | 10:C:452:LEU:N       | 2.69                     | 0.45              |
| 10:C:761:VAL:HG21    | 10:C:826:TYR:CA      | 2.42                     | 0.45              |
| 10:C:909:PRO:CB      | 10:C:920:LEU:HD22    | 2.46                     | 0.45              |
| 10:C8:1381:ALA:O     | 10:C8:1385:LEU:HB2   | 2.17                     | 0.45              |
| 18:B:245:LEU:HD21    | 18:B:268:GLN:NE2     | 2.32                     | 0.45              |
| 18:B:688:GLY:O       | 18:B:690:TRP:N       | 2.49                     | 0.45              |
| 18:B:1065:LYS:C      | 18:B:1067:SER:H      | 2.20                     | 0.45              |
| 18:B8:690:TRP:HH2    | 18:B8:787:VAL:CG2    | 2.18                     | 0.45              |
| 18:B8:1061:ALA:HA    | 18:B8:1064:ILE:CD1   | 2.47                     | 0.45              |
| 18:B8:1209:LEU:CD2   | 18:B8:1238:PHE:HE1   | 2.29                     | 0.45              |
| 18:B8:1438:LEU:CD1   | 18:B8:1462:LEU:CD1   | 2.94                     | 0.45              |
| 18:B8:1531:TRP:CE3   | 18:B8:1532:PHE:HA    | 2.52                     | 0.45              |
| 20:E:274:PRO:HA      | 20:E:279:GLN:OE1     | 2.15                     | 0.45              |
| 21:H:228:LEU:CD2     | 23:J32:592:VAL:CG1   | 2.92                     | 0.45              |
| 22:I24:303:SER:O     | 22:I24:307:VAL:HG23  | 2.16                     | 0.45              |
| 22:I24:332:MET:CG    | 23:J24:732:MET:HE1   | 2.46                     | 0.45              |
| 24:D:400:VAL:CG1     | 24:D16:751:MET:HB3   | 2.29                     | 0.45              |
| 24:D40:122:GLN:HE22  | 24:D40:151:VAL:HG21  | 1.82                     | 0.45              |
| 24:D40:749:ARG:NH2   | 24:D40:965:ASP:CG    | 2.75                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:62:ILE:HD13   | 10:C32:95:VAL:HG21   | 1.97                     | 0.45              |
| 10:C32:1530:PHE:CE1  | 12:A48:132:MET:CE    | 2.92                     | 0.45              |
| 10:C32:1708:ARG:HB2  | 10:C32:1730:ILE:HD13 | 1.98                     | 0.45              |
| 12:A48:823:VAL:O     | 12:A48:830:ILE:CD1   | 2.64                     | 0.45              |
| 1:R:422:ARG:HH21     | 1:R:580:GLU:CD       | 2.25                     | 0.45              |
| 1:R:1101:ARG:NE      | 24:D:1459:LEU:O      | 2.50                     | 0.45              |
| 1:R:1124:TRP:HH2     | 4:T:669:PRO:HA       | 1.82                     | 0.45              |
| 1:R:1328:LYS:HE3     | 10:C:1177:ARG:HE     | 1.75                     | 0.45              |
| 2:M:211:MET:HE3      | 3:N:280:ASN:CA       | 2.46                     | 0.45              |
| 2:M8:401:ARG:HD2     | 2:M8:487:TRP:CD1     | 2.52                     | 0.45              |
| 2:M8:783:TRP:O       | 8:L16:472:GLU:CD     | 2.59                     | 0.45              |
| 3:N8:9:GLY:C         | 3:N8:36:LYS:NZ       | 2.74                     | 0.45              |
| 1:R16:1112:LYS:HD3   | 5:P16:712:PHE:CZ     | 2.51                     | 0.45              |
| 2:M16:358:LEU:N      | 2:M16:359:PRO:CD     | 2.79                     | 0.45              |
| 2:M16:627:TYR:CB     | 3:N16:167:LEU:HA     | 2.47                     | 0.45              |
| 5:P:578:LEU:CD1      | 5:P:608:LYS:HZ2      | 2.30                     | 0.45              |
| 6:O:288:TRP:CE2      | 6:O:295:LEU:HD13     | 2.52                     | 0.45              |
| 5:P8:472:HIS:HB3     | 5:P8:475:THR:OG1     | 2.17                     | 0.45              |
| 5:P8:510:ILE:CD1     | 7:Q8:183:ARG:NH1     | 2.72                     | 0.45              |
| 7:Q16:183:ARG:HD3    | 7:Q16:229:ILE:CG2    | 2.46                     | 0.45              |
| 7:Q16:211:GLY:C      | 7:Q16:212:GLU:HG3    | 2.42                     | 0.45              |
| 7:Q16:306:MET:HE2    | 7:Q16:326:LEU:CD1    | 2.47                     | 0.45              |
| 9:K:727:ASP:C        | 9:K:729:VAL:N        | 2.73                     | 0.45              |
| 9:K:916:LYS:HA       | 9:K:919:MET:SD       | 2.57                     | 0.45              |
| 9:K8:955:TYR:CZ      | 9:K8:985:PHE:HA      | 2.50                     | 0.45              |
| 10:C16:460:TRP:CZ2   | 10:C16:495:LYS:HD2   | 2.51                     | 0.45              |
| 10:C16:1102:SER:C    | 10:C16:1104:GLN:H    | 2.24                     | 0.45              |
| 10:C16:1161:PHE:O    | 10:C16:1162:PRO:C    | 2.55                     | 0.45              |
| 10:C16:1285:VAL:CB   | 10:C16:1738:MET:CE   | 2.85                     | 0.45              |
| 10:C16:1381:ALA:O    | 10:C16:1385:LEU:HB2  | 2.16                     | 0.45              |
| 10:C16:1708:ARG:HB2  | 10:C16:1730:ILE:HD13 | 1.98                     | 0.45              |
| 10:C24:148:GLU:HA    | 10:C24:149:PRO:HD3   | 1.79                     | 0.45              |
| 10:C24:445:MET:HE1   | 10:C24:462:PHE:CE1   | 2.52                     | 0.45              |
| 10:C24:1164:VAL:HG13 | 10:C24:1167:PHE:HE2  | 1.81                     | 0.45              |
| 10:C24:1394:GLN:OE1  | 24:D24:1158:SER:CB   | 2.64                     | 0.45              |
| 10:C24:1424:GLN:HE22 | 10:C24:1478:VAL:HG13 | 1.81                     | 0.45              |
| 10:C24:1453:ARG:NH2  | 24:D24:1150:GLY:C    | 2.70                     | 0.45              |
| 12:A:126:ARG:HH11    | 10:C:1337:LEU:HD23   | 1.80                     | 0.45              |
| 12:A:696:ILE:CD1     | 12:A:725:GLY:HA2     | 2.47                     | 0.45              |
| 13:V:783:TRP:HZ2     | 14:W:671:GLU:CB      | 2.30                     | 0.45              |
| 13:V:800:LYS:HB3     | 14:W:688:HIS:CE1     | 2.51                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:J:722:LEU:HD13   | 10:C8:1623:ILE:HD11 | 1.95                     | 0.45              |
| 10:C8:68:LEU:HB3    | 10:C8:69:PRO:HD2    | 1.98                     | 0.45              |
| 10:C8:296:PHE:CE1   | 10:C8:300:VAL:CG2   | 3.00                     | 0.45              |
| 10:C8:1161:PHE:O    | 10:C8:1162:PRO:C    | 2.55                     | 0.45              |
| 10:C8:1713:ALA:O    | 10:C8:1717:ILE:HG13 | 2.16                     | 0.45              |
| 11:A16:506:TYR:CE1  | 11:A16:510:LEU:HD11 | 2.52                     | 0.45              |
| 18:B:32:LEU:CD1     | 18:B:163:ILE:CD1    | 2.83                     | 0.45              |
| 18:B:458:GLU:O      | 18:B:461:PHE:HB3    | 2.16                     | 0.45              |
| 18:B:530:SER:O      | 18:B:531:ASN:HB2    | 2.16                     | 0.45              |
| 18:B:729:LEU:CB     | 18:B:1196:MET:HE3   | 2.44                     | 0.45              |
| 18:B:1175:ALA:HA    | 18:B:1325:MET:CE    | 2.46                     | 0.45              |
| 18:B:1186:LEU:HD21  | 18:B:1199:VAL:HG13  | 1.97                     | 0.45              |
| 18:B:1275:TYR:OH    | 18:B:1300:GLU:OE2   | 2.25                     | 0.45              |
| 18:B8:268:GLN:HE21  | 18:B8:323:GLU:HB3   | 1.77                     | 0.45              |
| 18:B8:1094:MET:HE2  | 18:B8:1145:TRP:CH2  | 2.52                     | 0.45              |
| 20:E:353:ILE:CG2    | 20:E:413:PHE:CD2    | 2.87                     | 0.45              |
| 19:48:339:LEU:HA    | 24:D8:140:ALA:HB2   | 1.98                     | 0.45              |
| 20:E8:263:GLU:HB3   | 20:E8:264:PRO:HD3   | 1.98                     | 0.45              |
| 20:E8:355:PRO:O     | 20:E8:454:MET:HE1   | 2.16                     | 0.45              |
| 21:H8:338:MET:SD    | 22:I8:304:LEU:HD21  | 2.56                     | 0.45              |
| 21:H24:284:LEU:CD2  | 23:J24:647:MET:O    | 2.64                     | 0.45              |
| 22:I24:161:VAL:CG2  | 23:J24:585:LEU:HD21 | 2.46                     | 0.45              |
| 21:H16:232:LEU:CD1  | 22:I16:167:ILE:HG23 | 2.47                     | 0.45              |
| 22:I16:368:VAL:CG2  | 23:J16:591:LYS:HZ2  | 2.30                     | 0.45              |
| 24:D:393:LEU:HD11   | 24:D16:744:LEU:HD21 | 1.98                     | 0.45              |
| 24:D8:122:GLN:HE22  | 24:D8:151:VAL:HG21  | 1.82                     | 0.45              |
| 24:D8:552:VAL:HG21  | 24:D8:592:ILE:HD11  | 1.97                     | 0.45              |
| 24:D32:695:THR:HG22 | 24:D32:808:SER:OG   | 2.17                     | 0.45              |
| 10:C32:64:LEU:CD1   | 10:C32:70:ILE:HD12  | 2.42                     | 0.45              |
| 1:R:1328:LYS:CA     | 10:C:1173:LEU:HD21  | 2.33                     | 0.45              |
| 2:M:358:LEU:N       | 2:M:359:PRO:CD      | 2.79                     | 0.45              |
| 2:M:401:ARG:HD2     | 2:M:487:TRP:CD1     | 2.52                     | 0.45              |
| 2:M:673:ASN:CG      | 2:M:681:ALA:HB2     | 2.41                     | 0.45              |
| 1:R8:1428:VAL:HG13  | 1:R8:1431:ARG:HE    | 1.79                     | 0.45              |
| 1:R8:1438:TRP:NE1   | 3:N8:58:PRO:HG2     | 2.31                     | 0.45              |
| 1:R8:1486:SER:HA    | 2:M8:177:VAL:CG2    | 2.44                     | 0.45              |
| 2:M8:191:TRP:HH2    | 2:M8:222:ILE:HD11   | 1.82                     | 0.45              |
| 2:M8:552:PHE:CZ     | 2:M8:559:PHE:HE2    | 2.20                     | 0.45              |
| 5:P:158:VAL:HG11    | 5:P:248:ILE:HG23    | 1.98                     | 0.45              |
| 5:P:472:HIS:HB3     | 5:P:475:THR:OG1     | 2.17                     | 0.45              |
| 6:O:288:TRP:CZ3     | 6:O:315:TRP:CH2     | 3.05                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 7:Q:211:GLY:C        | 7:Q:212:GLU:HG3      | 2.42                     | 0.45              |
| 5:P8:614:VAL:HG21    | 5:P8:625:GLU:HG2     | 1.60                     | 0.45              |
| 5:P16:39:LEU:HD11    | 6:O16:323:PRO:HG2    | 1.98                     | 0.45              |
| 5:P16:641:GLN:HE22   | 5:P16:681:ALA:CB     | 2.29                     | 0.45              |
| 9:K8:909:ASP:OD1     | 9:K8:957:ILE:HD11    | 2.17                     | 0.45              |
| 9:K16:955:TYR:OH     | 9:K16:984:GLY:HA2    | 2.16                     | 0.45              |
| 9:K16:1248:LEU:HD11  | 9:K16:1265:ILE:HD12  | 1.97                     | 0.45              |
| 10:C16:68:LEU:HB3    | 10:C16:69:PRO:HD2    | 1.98                     | 0.45              |
| 10:C16:456:ASN:HB3   | 10:C16:459:LEU:HB2   | 1.99                     | 0.45              |
| 10:C16:1654:LEU:HD22 | 10:C16:1670:PRO:O    | 2.16                     | 0.45              |
| 11:A24:464:GLY:C     | 11:A24:466:SER:N     | 2.74                     | 0.45              |
| 11:A24:803:PRO:HA    | 24:D8:1401:LEU:CD1   | 2.47                     | 0.45              |
| 10:C24:460:TRP:CZ2   | 10:C24:495:LYS:HD2   | 2.51                     | 0.45              |
| 10:C24:1328:PHE:CZ   | 10:C24:1377:ILE:CD1  | 2.91                     | 0.45              |
| 10:C24:1488:ILE:HD13 | 10:C24:1528:LEU:HD23 | 1.99                     | 0.45              |
| 10:C24:1708:ARG:NH1  | 21:H24:279:GLU:HG3   | 2.29                     | 0.45              |
| 11:A40:464:GLY:C     | 11:A40:466:SER:N     | 2.74                     | 0.45              |
| 12:A:388:VAL:CG1     | 12:A:392:SER:HB2     | 2.46                     | 0.45              |
| 14:W:210:PRO:HA      | 14:W:219:ILE:CD1     | 2.47                     | 0.45              |
| 10:C:57:VAL:HG22     | 10:C:62:ILE:CD1      | 2.47                     | 0.45              |
| 10:C:664:ASN:OD1     | 10:C:697:HIS:HB2     | 2.17                     | 0.45              |
| 10:C:1713:ALA:O      | 10:C:1717:ILE:HG13   | 2.16                     | 0.45              |
| 10:C8:837:ARG:NH2    | 10:C8:890:ASP:O      | 2.48                     | 0.45              |
| 10:C8:847:ARG:HH22   | 10:C8:912:THR:H      | 1.63                     | 0.45              |
| 10:C8:1821:VAL:CG1   | 16:A8:144:LYS:CE     | 2.93                     | 0.45              |
| 11:A16:440:LEU:O     | 11:A16:443:LEU:HD12  | 2.16                     | 0.45              |
| 11:A16:587:VAL:HG21  | 11:A16:636:PHE:CE1   | 2.41                     | 0.45              |
| 11:A16:587:VAL:CG2   | 11:A16:627:ILE:HD13  | 2.47                     | 0.45              |
| 18:B:140:GLN:NE2     | 18:B:206:GLU:CD      | 2.62                     | 0.45              |
| 18:B:1438:LEU:CD1    | 18:B:1462:LEU:CD1    | 2.94                     | 0.45              |
| 18:B:1531:TRP:CE3    | 18:B:1532:PHE:HA     | 2.52                     | 0.45              |
| 18:B8:467:ILE:HG23   | 18:B8:581:LEU:HD22   | 1.99                     | 0.45              |
| 18:B8:1529:GLU:CD    | 24:D32:1415:LEU:HG   | 2.39                     | 0.45              |
| 20:E8:432:ILE:CG1    | 24:D40:72:GLU:HG2    | 2.44                     | 0.45              |
| 22:I:171:MET:HE1     | 23:J32:595:THR:OG1   | 2.16                     | 0.45              |
| 21:H8:232:LEU:CD1    | 22:I8:167:ILE:HG23   | 2.47                     | 0.45              |
| 21:H24:338:MET:SD    | 22:I24:304:LEU:HD21  | 2.56                     | 0.45              |
| 10:C32:33:ILE:HG22   | 10:C32:158:LEU:CD2   | 2.47                     | 0.45              |
| 10:C32:41:GLN:HE21   | 10:C32:165:ALA:HB1   | 1.82                     | 0.45              |
| 10:C32:68:LEU:HB3    | 10:C32:69:PRO:HD2    | 1.98                     | 0.45              |
| 10:C32:1594:PRO:CB   | 10:C32:1645:PHE:CD1  | 3.00                     | 0.45              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 12:A48:440:LEU:O    | 12:A48:443:LEU:HD12  | 2.16                     | 0.45              |
| 1:R:1362:ASP:O      | 1:R:1365:ILE:HG22    | 2.17                     | 0.45              |
| 2:M:552:PHE:CZ      | 2:M:559:PHE:HE2      | 2.20                     | 0.45              |
| 2:M:562:PHE:CE2     | 3:N:295:GLU:CD       | 2.95                     | 0.45              |
| 2:M8:816:ARG:CB     | 2:M8:850:TYR:CD2     | 3.00                     | 0.45              |
| 2:M8:851:LEU:CD2    | 4:T8:653:GLN:CG      | 2.85                     | 0.45              |
| 1:R16:1434:VAL:HG21 | 3:N16:151:VAL:O      | 2.15                     | 0.45              |
| 2:M16:225:ASP:CB    | 2:M16:606:GLN:HE22   | 2.28                     | 0.45              |
| 2:M16:544:LEU:HD12  | 2:M16:586:ALA:O      | 2.09                     | 0.45              |
| 2:M16:622:ARG:CZ    | 2:M16:624:ASP:OD2    | 2.64                     | 0.45              |
| 3:N16:1:MET:O       | 3:N16:302:PRO:C      | 2.60                     | 0.45              |
| 6:O:54:VAL:CG1      | 6:O:85:TRP:HE1       | 2.15                     | 0.45              |
| 7:Q:306:MET:HE2     | 7:Q:326:LEU:CD1      | 2.47                     | 0.45              |
| 5:P8:201:ILE:HD12   | 5:P8:211:TYR:CZ      | 2.51                     | 0.45              |
| 7:Q8:290:ASP:OD2    | 7:Q8:293:THR:OG1     | 2.27                     | 0.45              |
| 9:K8:1249:MET:HA    | 9:K8:1254:PHE:CG     | 2.51                     | 0.45              |
| 9:K16:912:TYR:CG    | 9:K16:957:ILE:HD11   | 2.52                     | 0.45              |
| 10:C16:490:GLN:HE21 | 10:C16:561:ASN:HB2   | 1.82                     | 0.45              |
| 10:C16:1215:ALA:HA  | 10:C16:1219:ILE:HD12 | 1.99                     | 0.45              |
| 11:A24:506:TYR:CE1  | 11:A24:510:LEU:HD11  | 2.52                     | 0.45              |
| 10:C24:57:VAL:HG22  | 10:C24:62:ILE:CD1    | 2.47                     | 0.45              |
| 10:C24:931:PRO:O    | 10:C24:939:LYS:HD2   | 2.16                     | 0.45              |
| 10:C24:1215:ALA:HA  | 10:C24:1219:ILE:HD12 | 1.99                     | 0.45              |
| 10:C24:1332:GLN:O   | 10:C24:1366:GLN:NE2  | 2.50                     | 0.45              |
| 10:C24:1708:ARG:HB2 | 10:C24:1730:ILE:HD13 | 1.99                     | 0.45              |
| 11:A40:696:ILE:CD1  | 11:A40:725:GLY:HA2   | 2.47                     | 0.45              |
| 14:W:628:HIS:CG     | 14:W:632:ILE:HD12    | 2.52                     | 0.45              |
| 10:C:1304:VAL:CG1   | 10:C:1384:ILE:HD11   | 2.45                     | 0.45              |
| 10:C:1624:LEU:HD22  | 10:C:1632:LEU:HD12   | 1.99                     | 0.45              |
| 10:C8:969:ASN:OD1   | 10:C8:979:MET:HE2    | 2.17                     | 0.45              |
| 10:C8:1708:ARG:CG   | 10:C8:1730:ILE:CD1   | 2.94                     | 0.45              |
| 18:B:1028:LYS:HE2   | 18:B:1032:GLN:NE2    | 2.32                     | 0.45              |
| 18:B:1161:LEU:CG    | 18:B:1403:ILE:CD1    | 2.95                     | 0.45              |
| 18:B:1658:MET:HE3   | 18:B:1662:TYR:HE2    | 1.81                     | 0.45              |
| 18:B8:334:PHE:CE1   | 18:B8:338:ILE:HD12   | 2.52                     | 0.45              |
| 18:B8:1119:LYS:C    | 18:B8:1120:THR:O     | 2.59                     | 0.45              |
| 18:B8:1142:PHE:CZ   | 18:B8:1348:VAL:HG12  | 2.52                     | 0.45              |
| 18:B8:1700:LEU:HD21 | 18:B8:1833:PHE:CE2   | 2.51                     | 0.45              |
| 18:B8:1943:HIS:HB3  | 18:B8:1945:TYR:CE1   | 2.52                     | 0.45              |
| 21:H:149:HIS:CD2    | 23:J32:565:ALA:CB    | 3.00                     | 0.45              |
| 21:H:232:LEU:CD1    | 22:I:167:ILE:HG23    | 2.47                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:J24:686:MET:CE    | 23:J24:694:ARG:NE    | 2.67                     | 0.45              |
| 24:D24:695:THR:HG22  | 24:D24:808:SER:OG    | 2.17                     | 0.45              |
| 24:D24:1330:ARG:CZ   | 24:D32:719:ARG:NH1   | 2.80                     | 0.45              |
| 10:C32:172:ILE:HG23  | 10:C32:240:ILE:CD1   | 2.46                     | 0.45              |
| 10:C32:399:HIS:CG    | 10:C32:400:PRO:HD2   | 2.52                     | 0.45              |
| 10:C32:553:LEU:CD2   | 10:C32:595:THR:HG23  | 2.45                     | 0.45              |
| 10:C32:795:ASP:OD1   | 10:C32:796:LEU:N     | 2.49                     | 0.45              |
| 10:C32:832:LEU:HG    | 10:C32:834:GLN:OE1   | 2.17                     | 0.45              |
| 10:C32:1332:GLN:O    | 10:C32:1366:GLN:NE2  | 2.50                     | 0.45              |
| 1:R8:1265:PHE:HD2    | 5:P8:684:ARG:CZ      | 2.27                     | 0.45              |
| 3:N8:4:GLN:CD        | 3:N8:44:GLY:HA2      | 2.40                     | 0.45              |
| 3:N8:163:ALA:O       | 3:N8:164:PRO:C       | 2.51                     | 0.45              |
| 1:R16:422:ARG:HH21   | 1:R16:580:GLU:CD     | 2.25                     | 0.45              |
| 1:R16:1486:SER:HA    | 2:M16:177:VAL:CG2    | 2.43                     | 0.45              |
| 2:M16:762:LEU:CD2    | 2:M16:813:ASN:HD22   | 2.29                     | 0.45              |
| 4:T16:671:ILE:HD13   | 5:P16:699:SER:CA     | 2.46                     | 0.45              |
| 6:O:119:ARG:NH2      | 6:O:182:GLU:CB       | 2.76                     | 0.45              |
| 5:P16:483:LEU:HD21   | 5:P16:493:LEU:HD23   | 1.98                     | 0.45              |
| 8:L8:527:ILE:HD13    | 8:L8:568:PHE:CE1     | 2.51                     | 0.45              |
| 9:K:1279:GLU:O       | 9:K:1281:SER:N       | 2.49                     | 0.45              |
| 9:K8:631:VAL:HG12    | 9:K8:764:VAL:CB      | 2.33                     | 0.45              |
| 10:C16:445:MET:HE1   | 10:C16:462:PHE:CE1   | 2.52                     | 0.45              |
| 10:C16:1074:LEU:HB2  | 18:B:256:VAL:O       | 2.17                     | 0.45              |
| 10:C16:1708:ARG:CG   | 10:C16:1730:ILE:CD1  | 2.94                     | 0.45              |
| 10:C16:1823:GLN:O    | 10:C16:1827:THR:OG1  | 2.34                     | 0.45              |
| 10:C24:664:ASN:OD1   | 10:C24:697:HIS:HB2   | 2.17                     | 0.45              |
| 10:C24:918:PHE:HA    | 10:C24:927:THR:HG21  | 1.99                     | 0.45              |
| 10:C24:1624:LEU:HD22 | 10:C24:1632:LEU:HD12 | 1.99                     | 0.45              |
| 10:C24:1708:ARG:CG   | 10:C24:1730:ILE:CD1  | 2.94                     | 0.45              |
| 11:A40:359:GLU:OE2   | 11:A40:362:ARG:NH2   | 2.50                     | 0.45              |
| 11:A40:468:VAL:HG23  | 24:D32:1100:GLN:OE1  | 2.10                     | 0.45              |
| 11:A40:749:GLN:NE2   | 24:D24:1398:ARG:CZ   | 2.80                     | 0.45              |
| 14:W:590:LEU:HD13    | 14:W:641:GLU:OE2     | 2.00                     | 0.45              |
| 10:C:460:TRP:CZ2     | 10:C:495:LYS:HD2     | 2.51                     | 0.45              |
| 10:C:585:PRO:HA      | 10:C:586:PRO:HD3     | 1.90                     | 0.45              |
| 10:C:918:PHE:HA      | 10:C:927:THR:HG21    | 1.99                     | 0.45              |
| 10:C:1424:GLN:HE22   | 10:C:1478:VAL:HG13   | 1.81                     | 0.45              |
| 10:C8:57:VAL:HG22    | 10:C8:62:ILE:CD1     | 2.47                     | 0.45              |
| 10:C8:225:LEU:HD21   | 10:C8:388:TYR:CE2    | 2.51                     | 0.45              |
| 10:C8:664:ASN:OD1    | 10:C8:697:HIS:HB2    | 2.17                     | 0.45              |
| 10:C8:1708:ARG:HB2   | 10:C8:1730:ILE:HD13  | 1.98                     | 0.45              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 11:A32:587:VAL:HG22  | 11:A32:627:ILE:CD1  | 2.47                     | 0.45              |
| 11:A32:798:PHE:CE2   | 11:A32:809:VAL:HG21 | 2.52                     | 0.45              |
| 18:B:374:ILE:CG2     | 18:B:380:LEU:HD13   | 2.46                     | 0.45              |
| 18:B:958:ARG:HG3     | 18:B:1029:THR:HG23  | 1.96                     | 0.45              |
| 18:B:1025:ASP:OD1    | 18:B:1285:MET:HE3   | 2.17                     | 0.45              |
| 18:B:1349:LEU:HD22   | 18:B:1367:ILE:CD1   | 2.46                     | 0.45              |
| 18:B:1926:VAL:HG22   | 18:B:1961:TYR:CD1   | 2.52                     | 0.45              |
| 18:B8:1025:ASP:OD1   | 18:B8:1285:MET:HE3  | 2.17                     | 0.45              |
| 20:E:163:ILE:HG22    | 20:E:165:ARG:HG3    | 1.99                     | 0.45              |
| 19:48:251:ARG:NH2    | 19:48:254:LEU:CD2   | 2.79                     | 0.45              |
| 21:H:338:MET:SD      | 22:I:304:LEU:HD21   | 2.57                     | 0.45              |
| 22:I:155:PHE:CZ      | 22:I:159:ARG:HD2    | 2.51                     | 0.45              |
| 24:D16:387:LEU:HD21  | 24:D16:411:MET:HG2  | 1.98                     | 0.45              |
| 24:D16:695:THR:HG22  | 24:D16:808:SER:OG   | 2.17                     | 0.45              |
| 24:D32:387:LEU:HD21  | 24:D32:411:MET:HG2  | 1.98                     | 0.45              |
| 10:C32:26:ARG:HE     | 10:C32:151:LEU:HD13 | 1.82                     | 0.45              |
| 10:C32:490:GLN:HE21  | 10:C32:561:ASN:HB2  | 1.82                     | 0.45              |
| 10:C32:547:VAL:HG21  | 10:C32:587:TYR:CD2  | 2.52                     | 0.45              |
| 10:C32:837:ARG:NH2   | 10:C32:890:ASP:O    | 2.49                     | 0.45              |
| 12:A48:696:ILE:CD1   | 12:A48:725:GLY:HA2  | 2.47                     | 0.45              |
| 1:R:672:LYS:HZ2      | 1:R:842:ASP:CG      | 2.24                     | 0.45              |
| 3:N:200:MET:CE       | 3:N:203:PHE:CD2     | 2.96                     | 0.45              |
| 1:R8:1124:TRP:CZ2    | 4:T8:669:PRO:CD     | 2.99                     | 0.45              |
| 6:O:43:SER:CB        | 7:Q:45:ASP:OD2      | 2.65                     | 0.45              |
| 7:Q:279:LEU:HD13     | 7:Q:323:PRO:HB2     | 1.99                     | 0.45              |
| 5:P8:442:GLU:OE2     | 5:P8:446:HIS:CE1    | 2.70                     | 0.45              |
| 7:Q8:183:ARG:HD3     | 7:Q8:229:ILE:CG2    | 2.46                     | 0.45              |
| 8:L16:173:ASP:OD2    | 12:A48:783:PHE:CD1  | 2.70                     | 0.45              |
| 9:K:899:GLU:OE1      | 9:K:903:ARG:NH2     | 2.50                     | 0.45              |
| 9:K:1056:VAL:HG11    | 9:K:1059:ARG:HH21   | 1.82                     | 0.45              |
| 9:K:1249:MET:HA      | 9:K:1254:PHE:CG     | 2.51                     | 0.45              |
| 9:K8:1117:LEU:HD11   | 9:K8:1135:THR:CG2   | 2.43                     | 0.45              |
| 10:C16:398:SER:HA    | 10:C16:458:VAL:CG1  | 2.46                     | 0.45              |
| 10:C16:1541:PHE:O    | 10:C16:1543:GLU:N   | 2.50                     | 0.45              |
| 10:C16:1665:THR:HG23 | 10:C24:1601:TYR:O   | 2.16                     | 0.45              |
| 11:A24:587:VAL:CG2   | 11:A24:627:ILE:HD13 | 2.47                     | 0.45              |
| 11:A24:696:ILE:CD1   | 11:A24:725:GLY:HA2  | 2.47                     | 0.45              |
| 10:C24:286:ILE:HG21  | 10:C24:292:PHE:CE1  | 2.45                     | 0.45              |
| 12:A:641:ARG:C       | 12:A:685:ARG:HH22   | 2.23                     | 0.45              |
| 12:A:782:PRO:C       | 12:A:783:PHE:CG     | 2.93                     | 0.45              |
| 12:A:823:VAL:O       | 12:A:830:ILE:CD1    | 2.64                     | 0.45              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 14:W:586:ILE:HG13    | 15:J:572:ASP:HB3    | 1.99                     | 0.45              |
| 10:C8:988:GLN:HE21   | 10:C8:1064:PHE:HE1  | 1.60                     | 0.45              |
| 11:A16:11:THR:HG21   | 22:I:162:GLN:CD     | 2.41                     | 0.45              |
| 11:A32:359:GLU:OE2   | 11:A32:362:ARG:NH2  | 2.50                     | 0.45              |
| 18:B:7:VAL:HG12      | 18:B:8:ASP:N        | 2.31                     | 0.45              |
| 18:B:580:GLU:OE2     | 18:B:643:MET:SD     | 2.75                     | 0.45              |
| 18:B:1094:MET:HE2    | 18:B:1145:TRP:CH2   | 2.52                     | 0.45              |
| 18:B:1142:PHE:CZ     | 18:B:1348:VAL:HG12  | 2.52                     | 0.45              |
| 18:B:1943:HIS:HB3    | 18:B:1945:TYR:CE1   | 2.52                     | 0.45              |
| 18:B8:460:PRO:CB     | 18:B8:562:ARG:NH1   | 2.76                     | 0.45              |
| 18:B8:891:VAL:HG22   | 18:B8:945:LEU:HA    | 1.99                     | 0.45              |
| 18:B8:1522:LEU:HD22  | 18:B8:1531:TRP:CG   | 2.52                     | 0.45              |
| 19:4:286:TRP:CG      | 20:E:163:ILE:HG23   | 2.49                     | 0.45              |
| 22:I8:303:SER:O      | 22:I8:307:VAL:HG23  | 2.16                     | 0.45              |
| 21:H24:366:MET:HE3   | 22:I24:332:MET:CE   | 2.32                     | 0.45              |
| 22:I16:368:VAL:HG21  | 23:J16:591:LYS:HZ2  | 1.81                     | 0.45              |
| 23:J16:718:GLN:HG3   | 23:J16:737:TRP:CZ3  | 2.52                     | 0.45              |
| 24:D16:122:GLN:HE22  | 24:D16:151:VAL:HG21 | 1.81                     | 0.45              |
| 10:C32:363:PHE:CD2   | 10:C32:367:ASN:ND2  | 2.84                     | 0.45              |
| 10:C32:909:PRO:CB    | 10:C32:920:LEU:HD22 | 2.46                     | 0.45              |
| 10:C32:993:HIS:HA    | 10:C32:996:THR:OG1  | 2.16                     | 0.45              |
| 10:C32:1164:VAL:HG13 | 10:C32:1167:PHE:HE2 | 1.81                     | 0.45              |
| 10:C32:1823:GLN:O    | 10:C32:1827:THR:OG1 | 2.34                     | 0.45              |
| 12:A48:587:VAL:CG2   | 12:A48:627:ILE:HD13 | 2.47                     | 0.45              |
| 2:M:225:ASP:CB       | 2:M:606:GLN:HE22    | 2.28                     | 0.45              |
| 1:R8:422:ARG:HH21    | 1:R8:580:GLU:CD     | 2.25                     | 0.45              |
| 2:M8:627:TYR:CB      | 3:N8:167:LEU:HA     | 2.47                     | 0.45              |
| 2:M8:762:LEU:CD2     | 2:M8:813:ASN:HD22   | 2.29                     | 0.45              |
| 1:R16:1124:TRP:CH2   | 4:T16:669:PRO:CG    | 2.95                     | 0.45              |
| 1:R16:1362:ASP:O     | 1:R16:1365:ILE:HG22 | 2.17                     | 0.45              |
| 1:R16:1490:VAL:O     | 1:R16:1494:THR:OG1  | 2.35                     | 0.45              |
| 2:M16:552:PHE:CZ     | 2:M16:559:PHE:HE2   | 2.20                     | 0.45              |
| 5:P:418:CYS:HA       | 5:P:422:PHE:HD2     | 1.82                     | 0.45              |
| 6:O:120:LYS:HE3      | 10:C:1163:LEU:CD1   | 2.47                     | 0.45              |
| 5:P8:213:LYS:HE3     | 5:P8:357:CYS:SG     | 2.57                     | 0.45              |
| 8:L16:527:ILE:HD13   | 8:L16:568:PHE:CE1   | 2.52                     | 0.45              |
| 8:L16:608:PHE:CZ     | 8:L16:635:MET:HG2   | 2.52                     | 0.45              |
| 10:C16:1699:LYS:CE   | 23:J32:722:LEU:HD22 | 2.38                     | 0.45              |
| 10:C24:26:ARG:HE     | 10:C24:151:LEU:HD13 | 1.82                     | 0.45              |
| 10:C24:41:GLN:HE21   | 10:C24:165:ALA:HB1  | 1.82                     | 0.45              |
| 10:C24:605:GLU:H     | 10:C24:605:GLU:HG2  | 1.47                     | 0.45              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 12:A:259:ILE:HG23   | 12:A:276:LEU:HD22    | 1.96                     | 0.45              |
| 12:A:440:LEU:O      | 12:A:443:LEU:HD12    | 2.16                     | 0.45              |
| 14:W:370:VAL:HG21   | 14:W:474:ILE:CD1     | 2.46                     | 0.45              |
| 14:W:709:LEU:HD11   | 15:J:643:THR:CB      | 2.47                     | 0.45              |
| 10:C:16:LEU:HD22    | 10:C:139:ARG:HH12    | 1.81                     | 0.45              |
| 10:C:572:ILE:CG1    | 10:C:606:MET:CE      | 2.90                     | 0.45              |
| 10:C:667:ILE:HA     | 10:C:670:GLU:N       | 2.31                     | 0.45              |
| 10:C:931:PRO:O      | 10:C:939:LYS:HD2     | 2.16                     | 0.45              |
| 10:C8:26:ARG:HE     | 10:C8:151:LEU:HD13   | 1.82                     | 0.45              |
| 10:C8:41:GLN:HE21   | 10:C8:165:ALA:HB1    | 1.82                     | 0.45              |
| 10:C8:456:ASN:HB3   | 10:C8:459:LEU:HB2    | 1.99                     | 0.45              |
| 10:C8:585:PRO:HA    | 10:C8:586:PRO:HD3    | 1.90                     | 0.45              |
| 10:C8:1488:ILE:HD13 | 10:C8:1528:LEU:HD23  | 1.99                     | 0.45              |
| 11:A16:696:ILE:CD1  | 11:A16:725:GLY:HA2   | 2.47                     | 0.45              |
| 17:F:72:SER:C       | 17:F:74:ILE:H        | 2.24                     | 0.45              |
| 18:B:1177:LEU:HD22  | 18:B:1321:MET:SD     | 2.57                     | 0.45              |
| 18:B:1234:MET:CB    | 18:B:1235:PRO:HD3    | 2.47                     | 0.45              |
| 18:B:1522:LEU:HD22  | 18:B:1531:TRP:CG     | 2.52                     | 0.45              |
| 18:B:1529:GLU:CD    | 24:D16:1415:LEU:HD12 | 2.34                     | 0.45              |
| 18:B:1556:SER:O     | 18:B:1560:ILE:HG13   | 2.17                     | 0.45              |
| 18:B:1778:ALA:N     | 18:B:1779:PRO:CD     | 2.80                     | 0.45              |
| 18:B8:580:GLU:OE2   | 18:B8:643:MET:SD     | 2.75                     | 0.45              |
| 18:B8:1778:ALA:N    | 18:B8:1779:PRO:CD    | 2.80                     | 0.45              |
| 20:E:429:PRO:HG2    | 24:D:69:VAL:CG2      | 2.46                     | 0.45              |
| 20:E:494:ILE:HD13   | 20:E:507:LEU:CB      | 2.47                     | 0.45              |
| 22:I8:321:LYS:HZ3   | 23:J8:711:GLU:HB2    | 1.81                     | 0.45              |
| 22:I8:332:MET:CG    | 23:J8:732:MET:HE1    | 2.46                     | 0.45              |
| 22:I8:364:ALA:O     | 22:I8:368:VAL:HG23   | 2.17                     | 0.45              |
| 21:H24:373:MET:HE2  | 22:I24:343:ARG:NH1   | 2.32                     | 0.45              |
| 22:I16:161:VAL:CG2  | 23:J16:585:LEU:HD21  | 2.46                     | 0.45              |
| 24:D8:472:ILE:HD11  | 24:D8:539:THR:CG2    | 2.47                     | 0.45              |
| 24:D24:387:LEU:HD21 | 24:D24:411:MET:HG2   | 1.98                     | 0.45              |
| 10:C32:365:LEU:HD22 | 10:C32:370:ARG:NH2   | 2.32                     | 0.45              |
| 10:C32:470:HIS:CD2  | 10:C32:508:ILE:HD11  | 2.44                     | 0.45              |
| 10:C32:736:ILE:HD11 | 10:C32:794:LYS:HZ2   | 1.82                     | 0.45              |
| 10:C32:1102:SER:C   | 10:C32:1104:GLN:H    | 2.24                     | 0.45              |
| 2:M:417:ARG:C       | 8:L:346:TRP:HZ2      | 2.25                     | 0.44              |
| 2:M:816:ARG:CB      | 2:M:850:TYR:CD2      | 3.00                     | 0.44              |
| 3:N:4:GLN:CD        | 3:N:44:GLY:HA2       | 2.40                     | 0.44              |
| 1:R8:1490:VAL:O     | 1:R8:1494:THR:OG1    | 2.36                     | 0.44              |
| 3:N8:19:MET:CE      | 3:N8:23:GLY:CA       | 2.75                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:R16:1466:LYS:HG3   | 6:O16:160:LEU:HB3    | 2.00                     | 0.44              |
| 2:M16:816:ARG:CB     | 2:M16:850:TYR:CD2    | 3.00                     | 0.44              |
| 5:P:641:GLN:HE22     | 5:P:681:ALA:CB       | 2.29                     | 0.44              |
| 5:P8:1:MET:HA        | 5:P8:2:PRO:HD3       | 1.50                     | 0.44              |
| 6:O8:179:LYS:CE      | 6:O8:183:GLN:OE1     | 2.56                     | 0.44              |
| 5:P16:213:LYS:HE3    | 5:P16:357:CYS:SG     | 2.57                     | 0.44              |
| 6:O16:119:ARG:NH2    | 6:O16:182:GLU:CB     | 2.76                     | 0.44              |
| 6:O16:288:TRP:CE2    | 6:O16:295:LEU:HD13   | 2.52                     | 0.44              |
| 9:K8:595:PHE:CD2     | 9:K8:601:VAL:HG22    | 2.52                     | 0.44              |
| 10:C16:1385:LEU:HD23 | 10:C16:1389:ILE:CD1  | 2.47                     | 0.44              |
| 10:C16:1624:LEU:HD22 | 10:C16:1632:LEU:HD12 | 1.99                     | 0.44              |
| 10:C16:1763:LEU:HD13 | 10:C16:1825:LEU:HD23 | 1.99                     | 0.44              |
| 11:A24:798:PHE:CE2   | 11:A24:809:VAL:HG21  | 2.52                     | 0.44              |
| 10:C24:399:HIS:CG    | 10:C24:400:PRO:HD2   | 2.52                     | 0.44              |
| 10:C24:456:ASN:HB3   | 10:C24:459:LEU:HB2   | 1.99                     | 0.44              |
| 10:C24:1381:ALA:O    | 10:C24:1385:LEU:HB2  | 2.16                     | 0.44              |
| 11:A40:36:ASN:HD21   | 22:I16:293:LYS:HE3   | 1.76                     | 0.44              |
| 11:A40:629:LEU:HD22  | 11:A40:675:LEU:CD1   | 2.46                     | 0.44              |
| 13:V:814:MET:HE2     | 13:V:814:MET:HB3     | 1.78                     | 0.44              |
| 14:W:469:LEU:HD23    | 14:W:555:THR:HG21    | 1.99                     | 0.44              |
| 10:C:490:GLN:HE21    | 10:C:561:ASN:HB2     | 1.82                     | 0.44              |
| 10:C:659:PHE:O       | 10:C:663:ILE:HG12    | 2.17                     | 0.44              |
| 10:C:1352:GLN:HE22   | 10:C:1357:LEU:CD1    | 2.29                     | 0.44              |
| 10:C:1420:LEU:HD22   | 10:C:1471:TYR:CE2    | 2.52                     | 0.44              |
| 10:C8:33:ILE:HG22    | 10:C8:158:LEU:CD2    | 2.47                     | 0.44              |
| 10:C8:1215:ALA:O     | 10:C8:1219:ILE:HB    | 2.16                     | 0.44              |
| 11:A16:124:ASN:ND2   | 18:B:1562:LYS:HB3    | 2.33                     | 0.44              |
| 11:A16:696:ILE:HD11  | 11:A16:728:ILE:HD12  | 1.92                     | 0.44              |
| 11:A32:11:THR:HG21   | 22:I24:162:GLN:CD    | 2.41                     | 0.44              |
| 11:A32:506:TYR:CE1   | 11:A32:510:LEU:HD11  | 2.52                     | 0.44              |
| 11:A32:587:VAL:CG2   | 11:A32:627:ILE:HD13  | 2.47                     | 0.44              |
| 18:B:349:PHE:CE1     | 18:B:353:ILE:HD12    | 2.44                     | 0.44              |
| 18:B:583:ARG:CD      | 18:B:643:MET:SD      | 3.05                     | 0.44              |
| 18:B:1679:ARG:C      | 18:B:1681:GLN:H      | 2.25                     | 0.44              |
| 18:B8:90:ILE:CD1     | 18:B8:131:ILE:HG21   | 2.40                     | 0.44              |
| 18:B8:286:GLN:OE1    | 18:B8:443:PHE:CD2    | 2.70                     | 0.44              |
| 18:B8:1161:LEU:CG    | 18:B8:1403:ILE:CD1   | 2.95                     | 0.44              |
| 18:B8:1234:MET:N     | 18:B8:1235:PRO:HD2   | 2.33                     | 0.44              |
| 18:B8:1234:MET:CB    | 18:B8:1235:PRO:HD3   | 2.47                     | 0.44              |
| 18:B8:1679:ARG:C     | 18:B8:1681:GLN:H     | 2.25                     | 0.44              |
| 18:B8:1926:VAL:HG22  | 18:B8:1961:TYR:CD1   | 2.52                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1947:GLU:N     | 18:B8:1948:PRO:HD2   | 2.33                     | 0.44              |
| 22:I:321:LYS:CE      | 23:J32:711:GLU:OE2   | 2.65                     | 0.44              |
| 21:H8:255:LEU:CD1    | 23:J8:655:GLU:CD     | 2.85                     | 0.44              |
| 21:H24:208:ASP:OD2   | 22:I24:142:ARG:NH2   | 2.50                     | 0.44              |
| 21:H24:228:LEU:CD2   | 23:J24:592:VAL:CG1   | 2.92                     | 0.44              |
| 24:D8:695:THR:HG22   | 24:D8:808:SER:OG     | 2.17                     | 0.44              |
| 10:C32:319:ALA:HA    | 10:C32:392:LEU:HD11  | 1.97                     | 0.44              |
| 10:C32:573:GLU:OE1   | 10:C32:617:TYR:OH    | 2.32                     | 0.44              |
| 10:C32:808:PRO:HB2   | 10:C32:810:ASP:OD1   | 2.17                     | 0.44              |
| 10:C32:1215:ALA:HA   | 10:C32:1219:ILE:HD12 | 1.99                     | 0.44              |
| 10:C32:1420:LEU:HD22 | 10:C32:1471:TYR:CE2  | 2.52                     | 0.44              |
| 10:C32:1537:GLU:OE2  | 10:C32:1540:GLU:CD   | 2.59                     | 0.44              |
| 12:A48:506:TYR:CE1   | 12:A48:510:LEU:HD11  | 2.52                     | 0.44              |
| 2:M:401:ARG:HB2      | 2:M:487:TRP:CE3      | 2.52                     | 0.44              |
| 2:M:627:TYR:CB       | 3:N:167:LEU:HA       | 2.47                     | 0.44              |
| 1:R8:1139:ARG:HH11   | 1:R8:1157:ARG:NH1    | 2.14                     | 0.44              |
| 2:M8:211:MET:HE3     | 3:N8:280:ASN:CA      | 2.46                     | 0.44              |
| 3:N8:208:LYS:HB2     | 3:N8:241:TRP:CH2     | 2.53                     | 0.44              |
| 1:R16:1124:TRP:CZ2   | 4:T16:669:PRO:CD     | 2.99                     | 0.44              |
| 1:R16:1172:HIS:HA    | 1:R16:1173:PRO:HD3   | 1.87                     | 0.44              |
| 1:R16:1266:THR:CG2   | 5:P16:680:ILE:HG21   | 2.32                     | 0.44              |
| 6:O:280:GLN:O        | 6:O:301:ASP:HB3      | 2.18                     | 0.44              |
| 5:P8:159:ILE:HD11    | 5:P8:214:LEU:HB2     | 1.97                     | 0.44              |
| 6:O8:288:TRP:CZ3     | 6:O8:315:TRP:CH2     | 3.05                     | 0.44              |
| 7:Q8:298:SER:C       | 7:Q8:300:SER:N       | 2.75                     | 0.44              |
| 5:P16:1:MET:HA       | 5:P16:2:PRO:HD3      | 1.50                     | 0.44              |
| 5:P16:201:ILE:HD12   | 5:P16:211:TYR:OH     | 2.17                     | 0.44              |
| 5:P16:507:GLN:HE21   | 7:Q16:136:ARG:NH2    | 2.13                     | 0.44              |
| 8:L:527:ILE:HD13     | 8:L:568:PHE:CE1      | 2.52                     | 0.44              |
| 8:L8:175:ARG:HH12    | 12:A48:134:LYS:CG    | 2.29                     | 0.44              |
| 8:L8:1074:ARG:CB     | 9:K8:1089:LYS:CE     | 2.76                     | 0.44              |
| 8:L16:1026:ARG:CB    | 9:K16:1284:MET:HG2   | 2.45                     | 0.44              |
| 9:K:1066:ASP:O       | 9:K:1068:GLN:N       | 2.51                     | 0.44              |
| 9:K:1164:ARG:NH2     | 9:K:1242:SER:O       | 2.49                     | 0.44              |
| 9:K8:827:ILE:HG12    | 9:K8:885:ALA:HB3     | 1.99                     | 0.44              |
| 10:C16:238:TYR:CE2   | 10:C16:313:ILE:HD13  | 2.53                     | 0.44              |
| 10:C16:918:PHE:HA    | 10:C16:927:THR:HG21  | 1.99                     | 0.44              |
| 10:C24:729:SER:C     | 10:C24:731:GLN:H     | 2.24                     | 0.44              |
| 10:C24:971:ASP:O     | 10:C24:975:SER:HB3   | 2.18                     | 0.44              |
| 10:C24:1821:VAL:HB   | 11:A40:144:LYS:NZ    | 2.32                     | 0.44              |
| 11:A40:11:THR:CG2    | 22:I16:162:GLN:NE2   | 2.67                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A40:506:TYR:CE1   | 11:A40:510:LEU:HD11  | 2.52                     | 0.44              |
| 12:A:359:GLU:OE2     | 12:A:362:ARG:NH2     | 2.50                     | 0.44              |
| 10:C:33:ILE:HG22     | 10:C:158:LEU:CD2     | 2.47                     | 0.44              |
| 10:C:1215:ALA:O      | 10:C:1219:ILE:HB     | 2.16                     | 0.44              |
| 10:C8:238:TYR:CE2    | 10:C8:313:ILE:HD13   | 2.53                     | 0.44              |
| 10:C8:808:PRO:HB2    | 10:C8:810:ASP:OD1    | 2.17                     | 0.44              |
| 10:C8:1215:ALA:HA    | 10:C8:1219:ILE:HD12  | 1.99                     | 0.44              |
| 11:A16:464:GLY:C     | 11:A16:466:SER:N     | 2.74                     | 0.44              |
| 18:B:1807:PRO:O      | 18:B:1808:GLY:C      | 2.56                     | 0.44              |
| 18:B8:583:ARG:CD     | 18:B8:643:MET:SD     | 3.05                     | 0.44              |
| 18:B8:958:ARG:HG3    | 18:B8:1029:THR:HG23  | 1.96                     | 0.44              |
| 18:B8:1807:PRO:O     | 18:B8:1808:GLY:C     | 2.56                     | 0.44              |
| 20:E8:449:ARG:C      | 20:E8:452:GLY:H      | 2.26                     | 0.44              |
| 22:I:364:ALA:O       | 22:I:368:VAL:HG23    | 2.17                     | 0.44              |
| 21:H24:149:HIS:CD2   | 23:J24:565:ALA:CB    | 3.00                     | 0.44              |
| 21:H16:316:ILE:O     | 21:H16:316:ILE:CG2   | 2.65                     | 0.44              |
| 21:H16:338:MET:SD    | 22:I16:304:LEU:HD21  | 2.57                     | 0.44              |
| 22:I16:131:ARG:CG    | 23:J16:557:ARG:HH22  | 2.11                     | 0.44              |
| 24:D24:1330:ARG:HG3  | 24:D24:1332:GLU:H    | 1.82                     | 0.44              |
| 10:C32:296:PHE:CE1   | 10:C32:300:VAL:CG2   | 3.00                     | 0.44              |
| 10:C32:659:PHE:O     | 10:C32:663:ILE:HG12  | 2.17                     | 0.44              |
| 10:C32:667:ILE:HA    | 10:C32:670:GLU:N     | 2.31                     | 0.44              |
| 10:C32:729:SER:C     | 10:C32:731:GLN:H     | 2.24                     | 0.44              |
| 10:C32:1624:LEU:HD22 | 10:C32:1632:LEU:HD12 | 1.99                     | 0.44              |
| 1:R:1442:THR:HG21    | 3:N:13:ILE:HD11      | 1.77                     | 0.44              |
| 3:N:208:LYS:HB2      | 3:N:241:TRP:CH2      | 2.53                     | 0.44              |
| 1:R8:1124:TRP:HH2    | 4:T8:669:PRO:HA      | 1.81                     | 0.44              |
| 2:M16:401:ARG:HB2    | 2:M16:487:TRP:CE3    | 2.52                     | 0.44              |
| 2:M16:401:ARG:HD2    | 2:M16:487:TRP:CD1    | 2.52                     | 0.44              |
| 2:M16:625:HIS:CD2    | 3:N16:225:PRO:CB     | 2.98                     | 0.44              |
| 3:N16:18:GLN:HG3     | 3:N16:62:VAL:O       | 2.18                     | 0.44              |
| 5:P:317:ILE:HG23     | 5:P:342:LEU:HD22     | 2.00                     | 0.44              |
| 5:P8:201:ILE:HD12    | 5:P8:211:TYR:OH      | 2.17                     | 0.44              |
| 5:P8:418:CYS:HA      | 5:P8:422:PHE:HD2     | 1.82                     | 0.44              |
| 5:P16:418:CYS:HA     | 5:P16:422:PHE:HD2    | 1.82                     | 0.44              |
| 5:P16:604:TYR:CD2    | 5:P16:629:ARG:NH2    | 2.59                     | 0.44              |
| 6:O16:43:SER:CB      | 7:Q16:45:ASP:OD2     | 2.65                     | 0.44              |
| 9:K:827:ILE:HG12     | 9:K:885:ALA:HB3      | 1.99                     | 0.44              |
| 9:K:923:ILE:HG22     | 9:K:929:ARG:CZ       | 2.46                     | 0.44              |
| 9:K8:646:ILE:HA      | 9:K8:649:MET:HE2     | 1.98                     | 0.44              |
| 10:C16:57:VAL:HG22   | 10:C16:62:ILE:CD1    | 2.47                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C16:365:LEU:HD22 | 10:C16:370:ARG:NH2  | 2.32                     | 0.44              |
| 10:C16:453:LEU:CG   | 10:C16:486:LEU:HD21 | 2.48                     | 0.44              |
| 10:C16:659:PHE:O    | 10:C16:663:ILE:HG12 | 2.17                     | 0.44              |
| 10:C16:722:LEU:HA   | 10:C16:725:LEU:HD12 | 2.00                     | 0.44              |
| 10:C16:808:PRO:HB2  | 10:C16:810:ASP:OD1  | 2.17                     | 0.44              |
| 10:C16:1594:PRO:CB  | 10:C16:1645:PHE:CD1 | 3.00                     | 0.44              |
| 10:C24:238:TYR:CE2  | 10:C24:313:ILE:HD13 | 2.53                     | 0.44              |
| 10:C24:993:HIS:HA   | 10:C24:996:THR:OG1  | 2.16                     | 0.44              |
| 10:C24:1624:LEU:CD2 | 10:C24:1632:LEU:CD1 | 2.96                     | 0.44              |
| 11:A40:798:PHE:CE2  | 11:A40:809:VAL:HG21 | 2.52                     | 0.44              |
| 12:A:136:LEU:HD23   | 10:C:1757:GLN:OE1   | 2.11                     | 0.44              |
| 12:A:139:ASP:OD2    | 10:C:1591:LYS:NZ    | 2.34                     | 0.44              |
| 14:W:648:ASN:O      | 14:W:652:ILE:HG13   | 2.16                     | 0.44              |
| 10:C8:144:ASP:CB    | 10:C8:147:LEU:HD12  | 2.44                     | 0.44              |
| 10:C8:365:LEU:HD22  | 10:C8:370:ARG:NH2   | 2.32                     | 0.44              |
| 10:C8:490:GLN:HE21  | 10:C8:561:ASN:HB2   | 1.82                     | 0.44              |
| 10:C8:1304:VAL:CG1  | 10:C8:1384:ILE:HD11 | 2.45                     | 0.44              |
| 10:C8:1352:GLN:NE2  | 10:C8:1357:LEU:HD12 | 2.32                     | 0.44              |
| 11:A32:124:ASN:ND2  | 18:B8:1562:LYS:HB3  | 2.33                     | 0.44              |
| 17:F24:72:SER:C     | 17:F24:74:ILE:H     | 2.24                     | 0.44              |
| 18:B:745:ILE:HG22   | 18:B:767:VAL:HG21   | 1.99                     | 0.44              |
| 18:B8:51:LEU:HD13   | 18:B8:139:ARG:NH2   | 2.33                     | 0.44              |
| 18:B8:491:VAL:CG1   | 18:B8:552:SER:HA    | 2.48                     | 0.44              |
| 18:B8:1652:PHE:HZ   | 18:B8:1700:LEU:HD12 | 1.81                     | 0.44              |
| 20:E:263:GLU:HB3    | 20:E:264:PRO:HD3    | 1.98                     | 0.44              |
| 20:E8:163:ILE:HG22  | 20:E8:165:ARG:HG3   | 1.99                     | 0.44              |
| 20:E8:476:PHE:CG    | 20:E8:493:TRP:HH2   | 2.35                     | 0.44              |
| 21:H8:267:LYS:NZ    | 23:J8:634:SER:HB3   | 2.33                     | 0.44              |
| 22:I8:321:LYS:CE    | 23:J8:711:GLU:OE2   | 2.65                     | 0.44              |
| 21:H24:267:LYS:NZ   | 23:J24:634:SER:HB3  | 2.33                     | 0.44              |
| 22:I24:203:GLN:NE2  | 22:I24:209:TRP:HE1  | 2.15                     | 0.44              |
| 22:I24:364:ALA:O    | 22:I24:368:VAL:HG23 | 2.17                     | 0.44              |
| 22:I16:304:LEU:HB3  | 22:I16:305:PRO:CD   | 2.43                     | 0.44              |
| 22:I16:321:LYS:CE   | 23:J16:711:GLU:OE2  | 2.65                     | 0.44              |
| 10:C32:16:LEU:HD22  | 10:C32:139:ARG:HH12 | 1.80                     | 0.44              |
| 10:C32:398:SER:HA   | 10:C32:458:VAL:CG1  | 2.46                     | 0.44              |
| 10:C32:1381:ALA:O   | 10:C32:1385:LEU:HB2 | 2.16                     | 0.44              |
| 2:M8:399:THR:HB     | 2:M8:480:ARG:HE     | 1.83                     | 0.44              |
| 1:R16:526:ASN:O     | 1:R16:529:HIS:CE1   | 2.71                     | 0.44              |
| 2:M16:399:THR:HB    | 2:M16:480:ARG:HE    | 1.83                     | 0.44              |
| 5:P:43:TRP:CH2      | 5:P:76:LEU:CD1      | 3.01                     | 0.44              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P:201:ILE:HD12     | 5:P:211:TYR:OH      | 2.17                     | 0.44              |
| 7:Q8:219:GLY:CA      | 7:Q8:221:TRP:CD1    | 3.01                     | 0.44              |
| 7:Q8:306:MET:HE2     | 7:Q8:326:LEU:CD1    | 2.47                     | 0.44              |
| 5:P16:158:VAL:HG11   | 5:P16:248:ILE:HG23  | 1.98                     | 0.44              |
| 5:P16:159:ILE:HD11   | 5:P16:214:LEU:HB2   | 1.97                     | 0.44              |
| 5:P16:214:LEU:CD2    | 5:P16:236:VAL:HG12  | 2.45                     | 0.44              |
| 9:K16:1248:LEU:HD11  | 9:K16:1265:ILE:CD1  | 2.48                     | 0.44              |
| 10:C16:168:ARG:HH22  | 10:C16:227:ASP:C    | 2.23                     | 0.44              |
| 10:C16:664:ASN:OD1   | 10:C16:697:HIS:HB2  | 2.17                     | 0.44              |
| 10:C16:1164:VAL:HG13 | 10:C16:1167:PHE:HE2 | 1.81                     | 0.44              |
| 10:C16:1537:GLU:OE2  | 10:C16:1540:GLU:CD  | 2.60                     | 0.44              |
| 10:C16:1624:LEU:CD2  | 10:C16:1632:LEU:CD1 | 2.96                     | 0.44              |
| 11:A24:763:HIS:ND1   | 11:A24:815:VAL:HG21 | 2.33                     | 0.44              |
| 10:C24:363:PHE:CD2   | 10:C24:367:ASN:ND2  | 2.84                     | 0.44              |
| 10:C24:450:PRO:C     | 10:C24:452:LEU:N    | 2.69                     | 0.44              |
| 10:C24:722:LEU:HA    | 10:C24:725:LEU:HD12 | 2.00                     | 0.44              |
| 10:C24:1541:PHE:O    | 10:C24:1543:GLU:N   | 2.50                     | 0.44              |
| 10:C24:1770:LEU:O    | 10:C24:1836:LYS:NZ  | 2.51                     | 0.44              |
| 11:A40:737:GLU:CD    | 24:D32:871:ARG:HE   | 2.24                     | 0.44              |
| 10:C:300:VAL:HG12    | 10:C:317:ARG:HG2    | 1.99                     | 0.44              |
| 10:C:1069:TYR:HA     | 10:C:1070:PRO:HD3   | 1.65                     | 0.44              |
| 10:C:1332:GLN:O      | 10:C:1366:GLN:NE2   | 2.50                     | 0.44              |
| 10:C:1567:LEU:HA     | 10:C:1610:MET:HE1   | 2.00                     | 0.44              |
| 10:C8:16:LEU:HD22    | 10:C8:139:ARG:HH12  | 1.80                     | 0.44              |
| 10:C8:1082:ILE:O     | 10:C8:1084:LYS:N    | 2.51                     | 0.44              |
| 10:C8:1624:LEU:HD22  | 10:C8:1632:LEU:HD12 | 1.99                     | 0.44              |
| 11:A16:124:ASN:CA    | 18:B:1523:ARG:NH1   | 2.81                     | 0.44              |
| 11:A32:124:ASN:CA    | 18:B8:1523:ARG:NH1  | 2.80                     | 0.44              |
| 11:A32:696:ILE:CD1   | 11:A32:725:GLY:HA2  | 2.47                     | 0.44              |
| 17:F16:72:SER:C      | 17:F16:74:ILE:H     | 2.24                     | 0.44              |
| 18:B:609:TYR:HD2     | 18:B:610:VAL:HG23   | 1.75                     | 0.44              |
| 18:B:652:LEU:HD21    | 18:B:724:LEU:HD23   | 1.98                     | 0.44              |
| 18:B:1553:SER:OG     | 18:B:1556:SER:OG    | 2.35                     | 0.44              |
| 18:B:1697:LEU:CD1    | 18:B:1826:VAL:HG13  | 2.48                     | 0.44              |
| 18:B:1947:GLU:N      | 18:B:1948:PRO:HD2   | 2.33                     | 0.44              |
| 18:B8:745:ILE:HG22   | 18:B8:767:VAL:HG21  | 1.99                     | 0.44              |
| 18:B8:1028:LYS:HE2   | 18:B8:1032:GLN:NE2  | 2.32                     | 0.44              |
| 18:B8:1563:PHE:CE1   | 18:B8:1567:ILE:CD1  | 2.98                     | 0.44              |
| 20:E8:31:PHE:CE1     | 20:E8:46:PHE:HZ     | 2.36                     | 0.44              |
| 21:H:373:MET:HE2     | 22:I:343:ARG:NH1    | 2.32                     | 0.44              |
| 21:H8:149:HIS:CD2    | 23:J8:565:ALA:CB    | 3.00                     | 0.44              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 22:I24:203:GLN:CD   | 22:I24:209:TRP:HZ2   | 2.19                     | 0.44              |
| 22:I16:203:GLN:NE2  | 22:I16:209:TRP:HE1   | 2.15                     | 0.44              |
| 24:D16:1380:LEU:HB3 | 24:D16:1454:LEU:HD21 | 2.00                     | 0.44              |
| 24:D32:1380:LEU:HB3 | 24:D32:1454:LEU:HD21 | 2.00                     | 0.44              |
| 10:C32:1069:TYR:HA  | 10:C32:1070:PRO:HD3  | 1.65                     | 0.44              |
| 10:C32:1541:PHE:O   | 10:C32:1543:GLU:N    | 2.50                     | 0.44              |
| 10:C32:1567:LEU:HA  | 10:C32:1610:MET:HE1  | 2.00                     | 0.44              |
| 10:C32:1821:VAL:HB  | 12:A48:144:LYS:NZ    | 2.32                     | 0.44              |
| 2:M:225:ASP:O       | 2:M:228:VAL:HG22     | 2.18                     | 0.44              |
| 2:M8:732:TRP:CZ3    | 2:M8:736:ALA:HB3     | 2.53                     | 0.44              |
| 3:N8:18:GLN:HG3     | 3:N8:62:VAL:O        | 2.18                     | 0.44              |
| 3:N8:227:SER:HB2    | 3:N8:243:VAL:HG12    | 1.98                     | 0.44              |
| 1:R16:1201:LEU:O    | 1:R16:1202:ARG:C     | 2.56                     | 0.44              |
| 3:N16:97:HIS:CD2    | 3:N16:99:PHE:CZ      | 3.06                     | 0.44              |
| 5:P16:220:GLU:OE2   | 5:P16:232:ARG:NH2    | 2.49                     | 0.44              |
| 5:P16:472:HIS:HB3   | 5:P16:475:THR:OG1    | 2.17                     | 0.44              |
| 9:K8:719:GLY:CA     | 9:K8:720:SER:N       | 2.70                     | 0.44              |
| 9:K8:899:GLU:OE1    | 9:K8:903:ARG:NH2     | 2.50                     | 0.44              |
| 9:K8:1028:GLN:OE1   | 9:K8:1040:THR:OG1    | 2.31                     | 0.44              |
| 10:C16:399:HIS:CG   | 10:C16:400:PRO:HD2   | 2.52                     | 0.44              |
| 10:C16:971:ASP:O    | 10:C16:975:SER:HB3   | 2.18                     | 0.44              |
| 10:C16:1332:GLN:O   | 10:C16:1366:GLN:NE2  | 2.50                     | 0.44              |
| 10:C16:1567:LEU:HA  | 10:C16:1610:MET:HE1  | 2.00                     | 0.44              |
| 10:C16:1663:SER:O   | 10:C24:1568:ARG:NH2  | 2.50                     | 0.44              |
| 11:A24:156:MET:HA   | 11:A24:555:HIS:NE2   | 2.30                     | 0.44              |
| 11:A24:629:LEU:HD22 | 11:A24:675:LEU:CD1   | 2.46                     | 0.44              |
| 10:C24:832:LEU:HG   | 10:C24:834:GLN:OE1   | 2.17                     | 0.44              |
| 10:C24:1314:GLU:OE1 | 10:C24:1318:ARG:NH2  | 2.38                     | 0.44              |
| 10:C24:1530:PHE:CE1 | 11:A40:132:MET:CE    | 2.92                     | 0.44              |
| 11:A40:740:LEU:HD11 | 24:D32:703:SER:OG    | 2.18                     | 0.44              |
| 10:C:1594:PRO:CB    | 10:C:1645:PHE:CD1    | 3.00                     | 0.44              |
| 10:C8:450:PRO:C     | 10:C8:452:LEU:N      | 2.69                     | 0.44              |
| 10:C8:553:LEU:CD2   | 10:C8:595:THR:HG23   | 2.45                     | 0.44              |
| 10:C8:959:GLU:HG2   | 10:C8:1139:ARG:NE    | 2.31                     | 0.44              |
| 11:A16:105:LEU:HD22 | 18:B:1350:ILE:HD12   | 1.99                     | 0.44              |
| 11:A32:20:LEU:CD1   | 21:H24:346:THR:CG2   | 2.90                     | 0.44              |
| 11:A32:105:LEU:HD22 | 18:B8:1350:ILE:HD12  | 1.99                     | 0.44              |
| 11:A32:212:LYS:HE3  | 11:A32:585:MET:HE3   | 1.76                     | 0.44              |
| 11:A32:464:GLY:C    | 11:A32:466:SER:N     | 2.74                     | 0.44              |
| 18:B:684:ILE:C      | 18:B:686:LEU:N       | 2.73                     | 0.44              |
| 18:B:1061:ALA:HA    | 18:B:1064:ILE:CD1    | 2.47                     | 0.44              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B:1194:LEU:HD11   | 18:B:1311:TRP:CH2   | 2.52                     | 0.44              |
| 18:B8:1556:SER:O     | 18:B8:1560:ILE:HG13 | 2.18                     | 0.44              |
| 18:B8:1697:LEU:CD1   | 18:B8:1826:VAL:HG13 | 2.48                     | 0.44              |
| 19:4:105:VAL:HG12    | 19:4:412:SER:OG     | 2.18                     | 0.44              |
| 21:H24:232:LEU:CD1   | 22:I24:167:ILE:HG23 | 2.47                     | 0.44              |
| 22:I16:300:LEU:HD22  | 23:J16:689:LEU:CD2  | 2.42                     | 0.44              |
| 10:C32:225:LEU:HD21  | 10:C32:388:TYR:CE2  | 2.51                     | 0.44              |
| 10:C32:238:TYR:CE2   | 10:C32:313:ILE:HD13 | 2.53                     | 0.44              |
| 10:C32:1623:ILE:HG22 | 10:C32:1623:ILE:O   | 2.18                     | 0.44              |
| 1:R:526:ASN:O        | 1:R:529:HIS:CE1     | 2.71                     | 0.44              |
| 1:R:746:GLU:CD       | 1:R:835:ARG:HE      | 2.25                     | 0.44              |
| 1:R:979:GLN:HG2      | 24:D:1438:ALA:HB3   | 1.99                     | 0.44              |
| 1:R:1206:GLN:HA      | 1:R:1207:PRO:HD3    | 1.88                     | 0.44              |
| 1:R:1486:SER:HA      | 2:M:177:VAL:CG2     | 2.43                     | 0.44              |
| 2:M:666:GLU:HA       | 2:M:684:GLN:OE1     | 2.18                     | 0.44              |
| 3:N:97:HIS:CD2       | 3:N:99:PHE:CZ       | 3.06                     | 0.44              |
| 3:N:158:TRP:CE3      | 3:N:179:LEU:HD21    | 2.51                     | 0.44              |
| 1:R8:1362:ASP:O      | 1:R8:1365:ILE:HG22  | 2.17                     | 0.44              |
| 2:M8:307:PHE:O       | 2:M8:311:GLN:HG2    | 2.18                     | 0.44              |
| 2:M8:625:HIS:CD2     | 3:N8:225:PRO:CB     | 2.98                     | 0.44              |
| 2:M8:820:LEU:C       | 2:M8:820:LEU:CD1    | 2.78                     | 0.44              |
| 3:N8:1:MET:O         | 3:N8:302:PRO:C      | 2.60                     | 0.44              |
| 3:N8:158:TRP:CE3     | 3:N8:179:LEU:HD21   | 2.51                     | 0.44              |
| 2:M16:307:PHE:O      | 2:M16:311:GLN:HG2   | 2.18                     | 0.44              |
| 2:M16:411:ILE:HD13   | 8:L16:393:TRP:CD1   | 2.52                     | 0.44              |
| 2:M16:732:TRP:CZ3    | 2:M16:736:ALA:HB3   | 2.53                     | 0.44              |
| 7:Q:10:VAL:CG2       | 7:Q:327:LEU:HD21    | 2.48                     | 0.44              |
| 7:Q:124:PHE:CE1      | 7:Q:125:TYR:CE2     | 2.80                     | 0.44              |
| 7:Q8:211:GLY:C       | 7:Q8:212:GLU:HG3    | 2.42                     | 0.44              |
| 5:P16:247:GLU:OE1    | 5:P16:295:LYS:CA    | 2.66                     | 0.44              |
| 5:P16:402:LEU:CD1    | 5:P16:433:LEU:HD22  | 2.46                     | 0.44              |
| 8:L8:976:LEU:HD21    | 9:K8:1004:ARG:CD    | 2.25                     | 0.44              |
| 9:K:806:LEU:HD12     | 9:K:874:VAL:CG1     | 2.44                     | 0.44              |
| 9:K:1051:GLU:O       | 9:K:1053:MET:N      | 2.48                     | 0.44              |
| 9:K8:923:ILE:HG23    | 9:K8:929:ARG:HE     | 1.75                     | 0.44              |
| 10:C16:41:GLN:HE21   | 10:C16:165:ALA:HB1  | 1.82                     | 0.44              |
| 10:C16:717:GLU:OE2   | 23:J8:656:ARG:HD2   | 2.17                     | 0.44              |
| 10:C16:1082:ILE:O    | 10:C16:1084:LYS:N   | 2.51                     | 0.44              |
| 10:C16:1708:ARG:NH1  | 21:H:276:GLY:HA2    | 2.33                     | 0.44              |
| 10:C24:33:ILE:HG22   | 10:C24:158:LEU:CD2  | 2.47                     | 0.44              |
| 10:C24:808:PRO:HB2   | 10:C24:810:ASP:OD1  | 2.17                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C24:1082:ILE:O    | 10:C24:1084:LYS:N    | 2.51                     | 0.44              |
| 10:C24:1537:GLU:OE2  | 10:C24:1540:GLU:CD   | 2.59                     | 0.44              |
| 12:A:144:LYS:NZ      | 10:C:1821:VAL:HB     | 2.32                     | 0.44              |
| 12:A:257:GLN:HG2     | 12:A:263:ASP:CG      | 2.43                     | 0.44              |
| 10:C8:453:LEU:CG     | 10:C8:486:LEU:HD21   | 2.48                     | 0.44              |
| 10:C8:1567:LEU:HA    | 10:C8:1610:MET:HE1   | 2.00                     | 0.44              |
| 11:A16:359:GLU:OE2   | 11:A16:362:ARG:NH2   | 2.49                     | 0.44              |
| 18:B:1068:THR:C      | 18:B:1070:GLY:H      | 2.25                     | 0.44              |
| 18:B8:171:ILE:CD1    | 18:B8:226:TYR:HB3    | 2.36                     | 0.44              |
| 18:B8:458:GLU:O      | 18:B8:461:PHE:HB3    | 2.17                     | 0.44              |
| 18:B8:583:ARG:HH11   | 18:B8:643:MET:HE1    | 1.79                     | 0.44              |
| 18:B8:938:LEU:CD2    | 18:B8:1019:ILE:HD13  | 2.48                     | 0.44              |
| 18:B8:1804:THR:O     | 18:B8:1805:GLU:C     | 2.55                     | 0.44              |
| 20:E:429:PRO:HD3     | 24:D:72:GLU:CB       | 2.47                     | 0.44              |
| 21:H:267:LYS:NZ      | 23:J32:634:SER:HB3   | 2.33                     | 0.44              |
| 23:J24:718:GLN:HG3   | 23:J24:737:TRP:CZ3   | 2.52                     | 0.44              |
| 21:H16:271:LEU:HD21  | 22:I16:254:ILE:HG21  | 1.98                     | 0.44              |
| 24:D24:1380:LEU:HB3  | 24:D24:1454:LEU:HD21 | 2.00                     | 0.44              |
| 10:C32:456:ASN:HB3   | 10:C32:459:LEU:HB2   | 1.99                     | 0.44              |
| 10:C32:1763:LEU:HD13 | 10:C32:1825:LEU:HD23 | 1.99                     | 0.44              |
| 10:C32:1767:LEU:CD1  | 10:C32:1832:MET:CE   | 2.96                     | 0.44              |
| 1:R:1169:ALA:HB1     | 5:P:701:ARG:NH1      | 2.33                     | 0.44              |
| 2:M:610:HIS:NE2      | 2:M:611:TRP:CD1      | 2.86                     | 0.44              |
| 2:M8:401:ARG:HB2     | 2:M8:487:TRP:CE3     | 2.52                     | 0.44              |
| 2:M16:544:LEU:CD2    | 2:M16:581:LEU:HD22   | 2.47                     | 0.44              |
| 5:P:213:LYS:HE3      | 5:P:357:CYS:SG       | 2.57                     | 0.44              |
| 5:P8:144:THR:C       | 5:P8:146:SER:H       | 2.22                     | 0.44              |
| 6:O8:43:SER:CB       | 7:Q8:45:ASP:OD2      | 2.65                     | 0.44              |
| 7:Q8:10:VAL:CG2      | 7:Q8:327:LEU:HD21    | 2.48                     | 0.44              |
| 7:Q8:279:LEU:HD13    | 7:Q8:323:PRO:HB2     | 1.99                     | 0.44              |
| 5:P16:68:GLY:HA3     | 6:O16:9:ASP:O        | 2.18                     | 0.44              |
| 6:O16:82:LEU:HD23    | 6:O16:103:MET:HE1    | 1.87                     | 0.44              |
| 7:Q16:10:VAL:CG2     | 7:Q16:327:LEU:HD21   | 2.48                     | 0.44              |
| 8:L8:956:ALA:HB1     | 8:L8:960:PHE:CE2     | 2.53                     | 0.44              |
| 9:K:700:MET:CE       | 9:K:764:VAL:HA       | 2.48                     | 0.44              |
| 9:K:842:ILE:HG23     | 9:K:871:LEU:CD2      | 2.48                     | 0.44              |
| 9:K:1117:LEU:HD11    | 9:K:1135:THR:CG2     | 2.43                     | 0.44              |
| 10:C16:26:ARG:HE     | 10:C16:151:LEU:HD13  | 1.82                     | 0.44              |
| 10:C16:33:ILE:HG22   | 10:C16:158:LEU:CD2   | 2.47                     | 0.44              |
| 10:C16:1457:LEU:HD23 | 10:C16:1521:ILE:HD13 | 2.00                     | 0.44              |
| 10:C16:1488:ILE:O    | 10:C16:1494:ILE:HD12 | 2.18                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:1623:ILE:HG22 | 10:C16:1623:ILE:O    | 2.18                     | 0.44              |
| 11:A24:103:GLU:CD    | 21:H8:323:TYR:OH     | 2.61                     | 0.44              |
| 11:A24:288:HIS:CB    | 11:A24:354:ARG:NH1   | 2.70                     | 0.44              |
| 11:A24:694:GLU:CD    | 24:D8:1398:ARG:HA    | 2.43                     | 0.44              |
| 10:C24:1763:LEU:HD13 | 10:C24:1825:LEU:HD23 | 1.99                     | 0.44              |
| 11:A40:762:ILE:CD1   | 11:A40:781:LEU:HD11  | 2.48                     | 0.44              |
| 12:A:506:TYR:CE1     | 12:A:510:LEU:HD11    | 2.52                     | 0.44              |
| 14:W:52:PRO:HD2      | 14:W:463:THR:HG23    | 2.00                     | 0.44              |
| 14:W:739:ARG:NH2     | 15:J:664:GLN:CG      | 2.81                     | 0.44              |
| 10:C:41:GLN:HE21     | 10:C:165:ALA:HB1     | 1.82                     | 0.44              |
| 10:C:808:PRO:HB2     | 10:C:810:ASP:OD1     | 2.17                     | 0.44              |
| 10:C:832:LEU:HG      | 10:C:834:GLN:OE1     | 2.17                     | 0.44              |
| 10:C:1352:GLN:NE2    | 10:C:1357:LEU:HD12   | 2.33                     | 0.44              |
| 10:C:1488:ILE:O      | 10:C:1494:ILE:HD12   | 2.18                     | 0.44              |
| 10:C:1708:ARG:HB2    | 10:C:1730:ILE:HD13   | 1.98                     | 0.44              |
| 10:C:1767:LEU:CD1    | 10:C:1832:MET:CE     | 2.96                     | 0.44              |
| 10:C8:918:PHE:HA     | 10:C8:927:THR:HG21   | 1.99                     | 0.44              |
| 10:C8:963:GLN:HE21   | 10:C8:967:GLU:HG2    | 1.83                     | 0.44              |
| 10:C8:1332:GLN:O     | 10:C8:1366:GLN:NE2   | 2.50                     | 0.44              |
| 10:C8:1541:PHE:O     | 10:C8:1543:GLU:N     | 2.50                     | 0.44              |
| 11:A16:212:LYS:HE3   | 11:A16:585:MET:HE3   | 1.77                     | 0.44              |
| 18:B:334:PHE:CE1     | 18:B:338:ILE:HD12    | 2.52                     | 0.44              |
| 18:B:491:VAL:CG1     | 18:B:552:SER:HA      | 2.48                     | 0.44              |
| 18:B:1668:PHE:CE2    | 18:B:1731:PHE:CD2    | 3.00                     | 0.44              |
| 18:B8:377:SER:C      | 18:B8:379:LEU:H      | 2.26                     | 0.44              |
| 19:48:105:VAL:HG12   | 19:48:412:SER:OG     | 2.18                     | 0.44              |
| 19:48:346:ILE:HG23   | 19:48:347:ALA:N      | 2.32                     | 0.44              |
| 21:H:228:LEU:HD22    | 23:J32:592:VAL:CG1   | 2.48                     | 0.44              |
| 22:I:332:MET:HG3     | 23:J32:732:MET:HE1   | 2.00                     | 0.44              |
| 21:H24:228:LEU:HD22  | 23:J24:592:VAL:CG1   | 2.48                     | 0.44              |
| 21:H16:322:LEU:CD1   | 23:J16:689:LEU:HG    | 2.46                     | 0.44              |
| 24:D:403:ARG:C       | 24:D16:748:GLU:OE1   | 2.60                     | 0.44              |
| 24:D:405:GLN:HA      | 24:D16:10:ARG:NH1    | 2.27                     | 0.44              |
| 24:D:695:THR:HG22    | 24:D:808:SER:OG      | 2.17                     | 0.44              |
| 24:D24:865:VAL:HG21  | 24:D24:885:TYR:HE1   | 1.83                     | 0.44              |
| 24:D32:94:ALA:HB1    | 24:D32:543:MET:HE1   | 2.00                     | 0.44              |
| 24:D40:695:THR:HG22  | 24:D40:808:SER:OG    | 2.17                     | 0.44              |
| 10:C32:971:ASP:O     | 10:C32:975:SER:HB3   | 2.18                     | 0.44              |
| 10:C32:1250:ALA:CB   | 10:C32:1309:ARG:HH12 | 2.15                     | 0.44              |
| 10:C32:1488:ILE:O    | 10:C32:1494:ILE:HD12 | 2.18                     | 0.44              |
| 10:C32:1560:GLN:OE1  | 10:C32:1601:TYR:HD1  | 1.96                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:1624:LEU:CD2  | 10:C32:1632:LEU:CD1  | 2.96                     | 0.44              |
| 12:A48:257:GLN:HG2   | 12:A48:263:ASP:CG    | 2.43                     | 0.44              |
| 12:A48:465:SER:C     | 12:A48:467:SER:N     | 2.72                     | 0.44              |
| 1:R:1124:TRP:HZ2     | 4:T:669:PRO:HD3      | 1.83                     | 0.44              |
| 2:M:421:LEU:CD1      | 8:L:346:TRP:NE1      | 2.80                     | 0.44              |
| 1:R8:1078:SER:OG     | 5:P8:713:LEU:HD21    | 2.14                     | 0.44              |
| 1:R8:1188:TYR:CE1    | 24:D40:1459:LEU:HD13 | 2.53                     | 0.44              |
| 2:M8:225:ASP:O       | 2:M8:228:VAL:HG22    | 2.18                     | 0.44              |
| 2:M8:363:ARG:NH1     | 2:M8:494:SER:C       | 2.71                     | 0.44              |
| 3:N8:19:MET:HG2      | 3:N8:23:GLY:HA2      | 2.00                     | 0.44              |
| 2:M16:225:ASP:O      | 2:M16:228:VAL:HG22   | 2.18                     | 0.44              |
| 5:P8:36:VAL:HG21     | 6:O8:323:PRO:HB2     | 1.99                     | 0.44              |
| 5:P8:454:GLY:O       | 5:P8:488:LYS:NZ      | 2.51                     | 0.44              |
| 5:P16:442:GLU:OE2    | 5:P16:446:HIS:CE1    | 2.70                     | 0.44              |
| 6:O16:280:GLN:O      | 6:O16:301:ASP:HB3    | 2.18                     | 0.44              |
| 8:L8:608:PHE:CG      | 8:L8:635:MET:SD      | 3.10                     | 0.44              |
| 8:L16:956:ALA:HB1    | 8:L16:960:PHE:CE2    | 2.53                     | 0.44              |
| 9:K:631:VAL:HG12     | 9:K:764:VAL:CB       | 2.33                     | 0.44              |
| 9:K:1063:GLU:O       | 9:K:1065:GLU:N       | 2.51                     | 0.44              |
| 10:C16:832:LEU:HG    | 10:C16:834:GLN:OE1   | 2.17                     | 0.44              |
| 10:C16:1307:ILE:HG12 | 10:C16:1320:GLN:HB3  | 2.00                     | 0.44              |
| 10:C24:1285:VAL:CB   | 10:C24:1738:MET:CE   | 2.85                     | 0.44              |
| 10:C24:1457:LEU:HD23 | 10:C24:1521:ILE:HD13 | 2.00                     | 0.44              |
| 10:C24:1619:PRO:HB2  | 10:C24:1621:LYS:HG3  | 2.00                     | 0.44              |
| 10:C:26:ARG:HE       | 10:C:151:LEU:HD13    | 1.82                     | 0.44              |
| 10:C:1082:ILE:O      | 10:C:1084:LYS:N      | 2.51                     | 0.44              |
| 10:C8:394:SER:HB3    | 10:C8:458:VAL:CB     | 2.48                     | 0.44              |
| 11:A32:257:GLN:HG2   | 11:A32:263:ASP:CG    | 2.43                     | 0.44              |
| 18:B:1205:ILE:HD12   | 18:B:1271:PHE:CE2    | 2.53                     | 0.44              |
| 18:B:1234:MET:N      | 18:B:1235:PRO:HD2    | 2.33                     | 0.44              |
| 18:B8:500:THR:O      | 18:B8:503:SER:OG     | 2.26                     | 0.44              |
| 18:B8:538:ARG:O      | 18:B8:545:VAL:HG13   | 2.18                     | 0.44              |
| 18:B8:731:ASN:OD1    | 18:B8:732:ASP:N      | 2.51                     | 0.44              |
| 19:4:346:ILE:HG23    | 19:4:347:ALA:N       | 2.32                     | 0.44              |
| 22:I24:332:MET:HG3   | 23:J24:732:MET:HE1   | 2.00                     | 0.44              |
| 21:H16:373:MET:HE2   | 22:I16:343:ARG:NH1   | 2.32                     | 0.44              |
| 24:D8:1380:LEU:HB3   | 24:D8:1454:LEU:HD21  | 2.00                     | 0.44              |
| 10:C32:722:LEU:HA    | 10:C32:725:LEU:HD12  | 2.00                     | 0.44              |
| 10:C32:1389:ILE:HD12 | 10:C32:1426:ARG:NH1  | 2.23                     | 0.44              |
| 10:C32:1488:ILE:HD13 | 10:C32:1528:LEU:HD23 | 1.99                     | 0.44              |
| 2:M:399:THR:HB       | 2:M:480:ARG:HE       | 1.83                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M:458:LYS:HE2      | 2:M:472:GLN:CD       | 2.43                     | 0.44              |
| 3:N:18:GLN:HG3       | 3:N:62:VAL:O         | 2.18                     | 0.44              |
| 3:N:97:HIS:HD2       | 3:N:99:PHE:CZ        | 2.36                     | 0.44              |
| 3:N:149:HIS:HD1      | 3:N:185:ASP:CG       | 2.26                     | 0.44              |
| 1:R8:1063:ARG:HE     | 24:D40:1432:THR:HG21 | 1.83                     | 0.44              |
| 1:R8:1139:ARG:NH1    | 1:R8:1157:ARG:NH1    | 2.63                     | 0.44              |
| 2:M8:762:LEU:HD22    | 2:M8:813:ASN:HD22    | 1.83                     | 0.44              |
| 3:N8:128:ASN:HB3     | 3:N8:144:ARG:HE      | 1.81                     | 0.44              |
| 2:M16:215:SER:OG     | 3:N16:7:GLU:OE1      | 2.34                     | 0.44              |
| 3:N16:19:MET:HG2     | 3:N16:23:GLY:HA2     | 1.99                     | 0.44              |
| 5:P:179:TYR:CE1      | 5:P:437:GLY:N        | 2.86                     | 0.44              |
| 5:P:442:GLU:OE2      | 5:P:446:HIS:CE1      | 2.70                     | 0.44              |
| 5:P:633:LEU:CD2      | 5:P:633:LEU:C        | 2.90                     | 0.44              |
| 7:Q:341:GLN:HA       | 10:C8:751:ARG:HH11   | 1.82                     | 0.44              |
| 5:P8:247:GLU:OE1     | 5:P8:295:LYS:CA      | 2.66                     | 0.44              |
| 5:P16:43:TRP:CH2     | 5:P16:76:LEU:CD1     | 3.01                     | 0.44              |
| 8:L:956:ALA:HB1      | 8:L:960:PHE:CE2      | 2.53                     | 0.44              |
| 9:K:646:ILE:HA       | 9:K:649:MET:HE2      | 1.98                     | 0.44              |
| 9:K:1034:PHE:HB2     | 9:K:1088:ASP:HB2     | 1.98                     | 0.44              |
| 9:K8:714:ARG:NH2     | 9:K8:729:VAL:O       | 2.48                     | 0.44              |
| 10:C16:1767:LEU:CD1  | 10:C16:1832:MET:CE   | 2.96                     | 0.44              |
| 10:C16:1770:LEU:O    | 10:C16:1836:LYS:NZ   | 2.51                     | 0.44              |
| 11:A24:24:ALA:O      | 23:J8:705:TRP:CZ2    | 2.70                     | 0.44              |
| 11:A24:107:GLN:HE22  | 21:H8:324:LEU:C      | 2.25                     | 0.44              |
| 11:A24:762:ILE:CD1   | 11:A24:781:LEU:HD11  | 2.48                     | 0.44              |
| 10:C24:585:PRO:HA    | 10:C24:586:PRO:HD3   | 1.90                     | 0.44              |
| 10:C24:659:PHE:O     | 10:C24:663:ILE:HG12  | 2.17                     | 0.44              |
| 10:C24:1002:LEU:HD23 | 10:C24:1012:ARG:NH2  | 2.31                     | 0.44              |
| 10:C24:1307:ILE:HG12 | 10:C24:1320:GLN:HB3  | 2.00                     | 0.44              |
| 10:C24:1333:HIS:CE1  | 10:C24:1337:LEU:HD23 | 2.38                     | 0.44              |
| 13:V:818:THR:HA      | 13:V:824:TRP:CD1     | 2.53                     | 0.44              |
| 10:C:365:LEU:HD22    | 10:C:370:ARG:NH2     | 2.32                     | 0.44              |
| 10:C:1424:GLN:HE22   | 10:C:1478:VAL:CG1    | 2.27                     | 0.44              |
| 10:C:1763:LEU:HD13   | 10:C:1825:LEU:HD23   | 1.99                     | 0.44              |
| 10:C:1770:LEU:O      | 10:C:1836:LYS:NZ     | 2.51                     | 0.44              |
| 10:C8:399:HIS:CG     | 10:C8:400:PRO:HD2    | 2.52                     | 0.44              |
| 10:C8:667:ILE:HA     | 10:C8:670:GLU:N      | 2.31                     | 0.44              |
| 10:C8:960:PHE:CZ     | 10:C8:1138:GLU:HB2   | 2.50                     | 0.44              |
| 10:C8:971:ASP:O      | 10:C8:975:SER:HB3    | 2.18                     | 0.44              |
| 10:C8:1420:LEU:HD22  | 10:C8:1471:TYR:CE2   | 2.52                     | 0.44              |
| 10:C8:1488:ILE:O     | 10:C8:1494:ILE:HD12  | 2.18                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C8:1624:LEU:CD2   | 10:C8:1632:LEU:CD1   | 2.96                     | 0.44              |
| 10:C8:1823:GLN:O     | 10:C8:1827:THR:OG1   | 2.33                     | 0.44              |
| 11:A32:504:TYR:HB3   | 11:A32:505:PRO:CD    | 2.46                     | 0.44              |
| 18:B:51:LEU:HD13     | 18:B:139:ARG:NH2     | 2.33                     | 0.44              |
| 18:B:1434:VAL:HG12   | 18:B:1438:LEU:HD12   | 1.99                     | 0.44              |
| 18:B8:684:ILE:C      | 18:B8:686:LEU:N      | 2.73                     | 0.44              |
| 18:B8:1068:THR:C     | 18:B8:1070:GLY:H     | 2.25                     | 0.44              |
| 18:B8:1649:SER:CA    | 18:B8:1653:LEU:HD12  | 2.44                     | 0.44              |
| 18:B8:1960:LEU:HD23  | 18:B8:1961:TYR:CE2   | 2.53                     | 0.44              |
| 20:E:14:ARG:NH2      | 20:E:244:LYS:O       | 2.50                     | 0.44              |
| 20:E8:347:PRO:HA     | 20:E8:348:PRO:HD3    | 1.76                     | 0.44              |
| 20:E8:353:ILE:CG1    | 20:E8:413:PHE:CD2    | 2.87                     | 0.44              |
| 22:I24:321:LYS:CE    | 23:J24:711:GLU:OE2   | 2.65                     | 0.44              |
| 24:D16:274:MET:HE3   | 24:D16:321:SER:CB    | 2.42                     | 0.44              |
| 24:D24:1452:LYS:HZ2  | 24:D32:971:HIS:CE1   | 2.30                     | 0.44              |
| 10:C32:1002:LEU:HD23 | 10:C32:1012:ARG:NH2  | 2.31                     | 0.44              |
| 10:C32:1257:ALA:C    | 10:C32:1323:LEU:HD11 | 2.43                     | 0.44              |
| 1:R:684:ASP:CG       | 1:R:784:TRP:HE1      | 2.26                     | 0.43              |
| 1:R:1437:VAL:HG12    | 1:R:1438:TRP:N       | 2.33                     | 0.43              |
| 2:M:544:LEU:HD21     | 2:M:586:ALA:CB       | 2.44                     | 0.43              |
| 1:R8:1124:TRP:HZ2    | 4:T8:669:PRO:HD3     | 1.83                     | 0.43              |
| 1:R8:1201:LEU:O      | 1:R8:1202:ARG:C      | 2.56                     | 0.43              |
| 2:M8:428:SER:CB      | 8:L8:355:SER:CB      | 2.91                     | 0.43              |
| 1:R16:1139:ARG:CG    | 1:R16:1157:ARG:NH1   | 2.77                     | 0.43              |
| 1:R16:1154:LEU:HD13  | 1:R16:1230:TYR:HA    | 2.00                     | 0.43              |
| 2:M16:217:ILE:HD11   | 3:N16:28:THR:CG2     | 2.43                     | 0.43              |
| 2:M16:339:GLU:C      | 2:M16:341:ASP:N      | 2.76                     | 0.43              |
| 6:O:133:LEU:HD11     | 6:O:153:PHE:CE1      | 2.48                     | 0.43              |
| 7:Q:136:ARG:NH1      | 7:Q:138:GLU:CD       | 2.76                     | 0.43              |
| 5:P8:68:GLY:HA3      | 6:O8:9:ASP:O         | 2.18                     | 0.43              |
| 5:P8:317:ILE:HG23    | 5:P8:342:LEU:HD22    | 2.00                     | 0.43              |
| 9:K:595:PHE:CD2      | 9:K:601:VAL:HG22     | 2.52                     | 0.43              |
| 9:K:649:MET:CB       | 9:K:704:ARG:HH22     | 2.06                     | 0.43              |
| 9:K8:587:LEU:HD23    | 9:K8:608:LEU:HD23    | 2.00                     | 0.43              |
| 10:C16:1085:SER:HB3  | 10:C16:1088:LEU:HD12 | 2.00                     | 0.43              |
| 10:C16:1480:PHE:CD1  | 24:D8:1407:PHE:CD2   | 3.06                     | 0.43              |
| 10:C16:1619:PRO:HB2  | 10:C16:1621:LYS:HG3  | 2.00                     | 0.43              |
| 11:A24:468:VAL:HG11  | 24:D16:1100:GLN:CA   | 2.48                     | 0.43              |
| 10:C24:365:LEU:HD22  | 10:C24:370:ARG:NH2   | 2.32                     | 0.43              |
| 10:C24:490:GLN:HE21  | 10:C24:561:ASN:HB2   | 1.82                     | 0.43              |
| 10:C24:1352:GLN:NE2  | 10:C24:1357:LEU:HD12 | 2.32                     | 0.43              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1594:PRO:CB  | 10:C24:1645:PHE:CD1  | 3.00                     | 0.43              |
| 13:V:818:THR:CG2    | 13:V:824:TRP:HE1     | 2.28                     | 0.43              |
| 10:C:296:PHE:CE1    | 10:C:300:VAL:CG2     | 3.00                     | 0.43              |
| 10:C:983:SER:HB3    | 10:C:1040:HIS:HD2    | 1.77                     | 0.43              |
| 10:C:1307:ILE:HG12  | 10:C:1320:GLN:HB3    | 2.00                     | 0.43              |
| 10:C8:643:LEU:HD11  | 10:C8:656:THR:OG1    | 2.17                     | 0.43              |
| 10:C8:764:ILE:HD13  | 10:C8:781:VAL:HG21   | 1.95                     | 0.43              |
| 18:B:891:VAL:HG22   | 18:B:945:LEU:HA      | 1.99                     | 0.43              |
| 18:B:1563:PHE:CE1   | 18:B:1567:ILE:CD1    | 2.98                     | 0.43              |
| 18:B:1662:TYR:CZ    | 18:B:1692:VAL:HG11   | 2.53                     | 0.43              |
| 18:B:1958:ALA:HB2   | 18:B:1965:LEU:HD12   | 2.00                     | 0.43              |
| 18:B8:1177:LEU:HD22 | 18:B8:1321:MET:SD    | 2.57                     | 0.43              |
| 18:B8:1434:VAL:HG12 | 18:B8:1438:LEU:HD12  | 1.99                     | 0.43              |
| 20:E:432:ILE:CG2    | 20:E:434:TRP:HD1     | 2.31                     | 0.43              |
| 19:48:94:VAL:O      | 19:48:97:LEU:HB2     | 2.18                     | 0.43              |
| 20:E8:432:ILE:CG2   | 20:E8:434:TRP:HD1    | 2.31                     | 0.43              |
| 23:J32:718:GLN:HG3  | 23:J32:737:TRP:CZ3   | 2.52                     | 0.43              |
| 21:H8:228:LEU:HD22  | 23:J8:592:VAL:CG1    | 2.48                     | 0.43              |
| 21:H8:316:ILE:O     | 21:H8:316:ILE:CG2    | 2.65                     | 0.43              |
| 21:H8:319:GLY:O     | 21:H8:321:SER:N      | 2.51                     | 0.43              |
| 22:I24:204:PRO:HA   | 22:I24:209:TRP:CZ3   | 2.53                     | 0.43              |
| 21:H16:267:LYS:NZ   | 23:J16:634:SER:HB3   | 2.33                     | 0.43              |
| 24:D24:865:VAL:HG21 | 24:D24:885:TYR:CE1   | 2.53                     | 0.43              |
| 10:C32:105:TRP:O    | 10:C32:106:GLY:O     | 2.36                     | 0.43              |
| 10:C32:453:LEU:HD22 | 10:C32:459:LEU:HD21  | 0.51                     | 0.43              |
| 10:C32:664:ASN:OD1  | 10:C32:697:HIS:HB2   | 2.17                     | 0.43              |
| 10:C32:667:ILE:HD11 | 10:C32:700:MET:HE2   | 1.82                     | 0.43              |
| 10:C32:1109:VAL:O   | 10:C32:1111:SER:N    | 2.51                     | 0.43              |
| 10:C32:1708:ARG:CA  | 10:C32:1730:ILE:HD11 | 2.48                     | 0.43              |
| 12:A48:763:HIS:ND1  | 12:A48:815:VAL:HG21  | 2.33                     | 0.43              |
| 12:A48:782:PRO:C    | 12:A48:783:PHE:CG    | 2.93                     | 0.43              |
| 1:R:1033:LYS:HZ3    | 24:D:1432:THR:HB     | 1.73                     | 0.43              |
| 2:M:250:LEU:HD23    | 2:M:287:TYR:CE2      | 2.53                     | 0.43              |
| 2:M:628:LEU:HD13    | 3:N:223:GLY:CA       | 2.39                     | 0.43              |
| 1:R8:684:ASP:CG     | 1:R8:784:TRP:HE1     | 2.26                     | 0.43              |
| 1:R8:1154:LEU:HD13  | 1:R8:1230:TYR:HA     | 2.00                     | 0.43              |
| 2:M8:161:ASP:OD1    | 2:M8:163:SER:OG      | 2.34                     | 0.43              |
| 3:N8:97:HIS:CD2     | 3:N8:99:PHE:CZ       | 3.06                     | 0.43              |
| 2:M16:428:SER:CB    | 8:L16:355:SER:CB     | 2.83                     | 0.43              |
| 3:N16:208:LYS:HB2   | 3:N16:241:TRP:CH2    | 2.53                     | 0.43              |
| 5:P:39:LEU:HD11     | 6:O:323:PRO:HG2      | 1.99                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P:633:LEU:HD23     | 5:P:639:THR:HG21     | 1.98                     | 0.43              |
| 6:O:236:PRO:O        | 6:O:240:ARG:NH2      | 2.49                     | 0.43              |
| 5:P8:43:TRP:CH2      | 5:P8:76:LEU:CD1      | 3.01                     | 0.43              |
| 5:P16:139:SER:O      | 5:P16:142:SER:OG     | 2.34                     | 0.43              |
| 5:P16:565:LEU:O      | 5:P16:568:SER:OG     | 2.35                     | 0.43              |
| 6:O16:288:TRP:CZ3    | 6:O16:315:TRP:CH2    | 3.05                     | 0.43              |
| 7:Q16:136:ARG:NH1    | 7:Q16:138:GLU:CD     | 2.76                     | 0.43              |
| 9:K:577:GLN:CD       | 9:K:625:ARG:NH1      | 2.76                     | 0.43              |
| 9:K8:1063:GLU:O      | 9:K8:1065:GLU:N      | 2.51                     | 0.43              |
| 9:K16:1214:TYR:CD2   | 9:K16:1232:LEU:HD21  | 2.53                     | 0.43              |
| 10:C16:148:GLU:HA    | 10:C16:149:PRO:HD3   | 1.79                     | 0.43              |
| 10:C16:196:ILE:CG2   | 10:C16:200:GLY:HA2   | 2.48                     | 0.43              |
| 10:C16:277:SER:O     | 10:C16:280:SER:N     | 2.36                     | 0.43              |
| 10:C16:1488:ILE:HD13 | 10:C16:1528:LEU:HD23 | 1.99                     | 0.43              |
| 11:A24:198:PRO:CB    | 11:A24:200:HIS:HE1   | 2.24                     | 0.43              |
| 10:C24:105:TRP:O     | 10:C24:106:GLY:O     | 2.36                     | 0.43              |
| 10:C24:280:SER:C     | 10:C24:282:LYS:N     | 2.74                     | 0.43              |
| 10:C24:510:TRP:HB2   | 10:C24:511:PRO:HD3   | 2.00                     | 0.43              |
| 10:C24:1271:PHE:CD1  | 10:C24:1273:GLY:N    | 2.81                     | 0.43              |
| 10:C24:1626:GLN:HE21 | 10:C24:1692:LYS:CE   | 2.31                     | 0.43              |
| 11:A40:390:ALA:HB1   | 24:D32:1099:ARG:CG   | 2.48                     | 0.43              |
| 14:W:349:ALA:O       | 14:W:447:MET:HE2     | 2.18                     | 0.43              |
| 14:W:742:VAL:HG21    | 15:J:668:ILE:HG23    | 2.00                     | 0.43              |
| 10:C:196:ILE:CG2     | 10:C:200:GLY:HA2     | 2.48                     | 0.43              |
| 10:C:399:HIS:CG      | 10:C:400:PRO:HD2     | 2.52                     | 0.43              |
| 10:C:453:LEU:CG      | 10:C:486:LEU:HD21    | 2.47                     | 0.43              |
| 10:C:547:VAL:HG21    | 10:C:587:TYR:CD2     | 2.52                     | 0.43              |
| 10:C:962:PHE:CE2     | 10:C:997:ILE:CD1     | 3.01                     | 0.43              |
| 10:C:971:ASP:O       | 10:C:975:SER:HB3     | 2.18                     | 0.43              |
| 10:C8:196:ILE:CG2    | 10:C8:200:GLY:HA2    | 2.48                     | 0.43              |
| 10:C8:659:PHE:O      | 10:C8:663:ILE:HG12   | 2.17                     | 0.43              |
| 10:C8:1109:VAL:O     | 10:C8:1111:SER:N     | 2.51                     | 0.43              |
| 10:C8:1594:PRO:CB    | 10:C8:1645:PHE:CD1   | 3.00                     | 0.43              |
| 10:C8:1725:THR:C     | 10:C8:1727:SER:H     | 2.26                     | 0.43              |
| 11:A16:257:GLN:HG2   | 11:A16:263:ASP:CG    | 2.43                     | 0.43              |
| 17:F:73:GLY:C        | 17:F:75:ALA:N        | 2.76                     | 0.43              |
| 18:B:286:GLN:OE1     | 18:B:443:PHE:CD2     | 2.70                     | 0.43              |
| 18:B:377:SER:C       | 18:B:379:LEU:H       | 2.26                     | 0.43              |
| 18:B:772:LYS:HE2     | 18:B:839:ASP:HB3     | 1.99                     | 0.43              |
| 18:B:938:LEU:CD2     | 18:B:1019:ILE:HD13   | 2.48                     | 0.43              |
| 18:B8:609:TYR:HD2    | 18:B8:610:VAL:HG23   | 1.75                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B8:1859:LEU:HB3   | 18:B8:1860:PRO:HD2   | 2.01                     | 0.43              |
| 20:E8:381:SER:O      | 20:E8:385:ASP:HB3    | 2.17                     | 0.43              |
| 21:H16:149:HIS:CD2   | 23:J16:565:ALA:CB    | 3.00                     | 0.43              |
| 22:I16:146:SER:HA    | 23:J16:571:TRP:CZ2   | 2.53                     | 0.43              |
| 24:D40:94:ALA:HB1    | 24:D40:543:MET:HE1   | 2.00                     | 0.43              |
| 10:C32:196:ILE:CG2   | 10:C32:200:GLY:HA2   | 2.48                     | 0.43              |
| 10:C32:510:TRP:HB2   | 10:C32:511:PRO:HD3   | 2.00                     | 0.43              |
| 10:C32:729:SER:C     | 10:C32:731:GLN:N     | 2.73                     | 0.43              |
| 2:M:627:TYR:CD2      | 2:M:627:TYR:N        | 2.85                     | 0.43              |
| 1:R8:746:GLU:CD      | 1:R8:835:ARG:HE      | 2.25                     | 0.43              |
| 2:M8:610:HIS:NE2     | 2:M8:611:TRP:CD1     | 2.86                     | 0.43              |
| 3:N8:169:SER:O       | 3:N8:170:SER:C       | 2.62                     | 0.43              |
| 1:R16:1075:LYS:CE    | 5:P16:713:LEU:O      | 2.56                     | 0.43              |
| 2:M16:610:HIS:NE2    | 2:M16:611:TRP:CD1    | 2.86                     | 0.43              |
| 5:P:62:ASP:N         | 5:P:62:ASP:OD1       | 2.49                     | 0.43              |
| 6:O8:280:GLN:O       | 6:O8:301:ASP:HB3     | 2.18                     | 0.43              |
| 7:Q8:51:ILE:HG12     | 7:Q8:121:ILE:HD11    | 1.98                     | 0.43              |
| 5:P16:281:ILE:HD11   | 5:P16:341:MET:CE     | 2.45                     | 0.43              |
| 9:K:577:GLN:CG       | 9:K:625:ARG:NH1      | 2.81                     | 0.43              |
| 9:K:959:TRP:CG       | 9:K:992:GLN:HG3      | 2.52                     | 0.43              |
| 9:K:1074:ARG:HH11    | 9:K:1126:LEU:CD2     | 2.30                     | 0.43              |
| 9:K8:646:ILE:HA      | 9:K8:649:MET:CE      | 2.48                     | 0.43              |
| 9:K8:745:ARG:CG      | 9:K8:752:MET:HA      | 2.48                     | 0.43              |
| 10:C16:1420:LEU:HD22 | 10:C16:1471:TYR:CE2  | 2.53                     | 0.43              |
| 10:C16:1708:ARG:CA   | 10:C16:1730:ILE:HD11 | 2.48                     | 0.43              |
| 11:A24:628:LEU:HG    | 11:A24:637:LEU:HD12  | 2.00                     | 0.43              |
| 10:C24:1109:VAL:O    | 10:C24:1111:SER:N    | 2.51                     | 0.43              |
| 11:A40:198:PRO:CB    | 11:A40:200:HIS:HE1   | 2.24                     | 0.43              |
| 11:A40:629:LEU:HD22  | 11:A40:675:LEU:HD12  | 2.01                     | 0.43              |
| 12:A:153:ARG:HA      | 10:C8:60:LYS:HE3     | 1.84                     | 0.43              |
| 13:V:861:PHE:CB      | 14:W:741:ARG:CZ      | 2.95                     | 0.43              |
| 10:C:238:TYR:CE2     | 10:C:313:ILE:HD13    | 2.53                     | 0.43              |
| 10:C:456:ASN:HB3     | 10:C:459:LEU:HB2     | 1.99                     | 0.43              |
| 10:C:555:LYS:HD3     | 10:C:555:LYS:HA      | 1.77                     | 0.43              |
| 10:C:750:TYR:OH      | 10:C:819:GLN:OE1     | 2.32                     | 0.43              |
| 10:C:1157:LEU:HD22   | 10:C:1176:VAL:HG11   | 2.01                     | 0.43              |
| 10:C:1257:ALA:C      | 10:C:1323:LEU:HD11   | 2.43                     | 0.43              |
| 10:C:1594:PRO:HG3    | 10:C:1642:TYR:CD2    | 2.54                     | 0.43              |
| 10:C8:1424:GLN:HE22  | 10:C8:1478:VAL:HG13  | 1.81                     | 0.43              |
| 10:C8:1770:LEU:O     | 10:C8:1836:LYS:NZ    | 2.51                     | 0.43              |
| 10:C8:1821:VAL:HB    | 16:A8:144:LYS:NZ     | 2.32                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:A16:375:ALA:N    | 11:A16:376:PRO:CD   | 2.81                     | 0.43              |
| 17:F8:73:GLY:C      | 17:F8:75:ALA:N      | 2.76                     | 0.43              |
| 11:A32:628:LEU:HG   | 11:A32:637:LEU:HD12 | 2.01                     | 0.43              |
| 17:F24:73:GLY:C     | 17:F24:75:ALA:N     | 2.76                     | 0.43              |
| 18:B:326:PRO:HG2    | 18:B:370:TYR:CD1    | 2.53                     | 0.43              |
| 18:B:520:ILE:HD11   | 18:B:528:ILE:HD11   | 2.00                     | 0.43              |
| 18:B:731:ASN:OD1    | 18:B:732:ASP:N      | 2.51                     | 0.43              |
| 18:B:1456:ASN:OD1   | 18:B:1510:TYR:HD1   | 2.01                     | 0.43              |
| 18:B8:192:PRO:HG2   | 18:B8:195:MET:SD    | 2.58                     | 0.43              |
| 18:B8:520:ILE:HD11  | 18:B8:528:ILE:HD11  | 2.00                     | 0.43              |
| 20:E:350:GLU:CG     | 20:E:352:PHE:HE2    | 2.30                     | 0.43              |
| 20:E:476:PHE:CG     | 20:E:493:TRP:HH2    | 2.35                     | 0.43              |
| 22:I:304:LEU:HB3    | 22:I:305:PRO:CD     | 2.43                     | 0.43              |
| 22:I8:97:THR:HG22   | 22:I8:107:THR:CG2   | 2.48                     | 0.43              |
| 22:I8:146:SER:HA    | 23:J8:571:TRP:CZ2   | 2.53                     | 0.43              |
| 21:H24:255:LEU:CD1  | 23:J24:655:GLU:CD   | 2.85                     | 0.43              |
| 22:I24:155:PHE:CZ   | 22:I24:159:ARG:HD2  | 2.52                     | 0.43              |
| 21:H16:228:LEU:HD22 | 23:J16:592:VAL:CG1  | 2.48                     | 0.43              |
| 22:I16:204:PRO:HA   | 22:I16:209:TRP:CZ3  | 2.53                     | 0.43              |
| 22:I16:364:ALA:O    | 22:I16:368:VAL:HG23 | 2.17                     | 0.43              |
| 24:D:472:ILE:HD11   | 24:D:539:THR:CG2    | 2.48                     | 0.43              |
| 24:D32:122:GLN:HE22 | 24:D32:151:VAL:HG21 | 1.81                     | 0.43              |
| 24:D32:472:ILE:HD11 | 24:D32:539:THR:CG2  | 2.48                     | 0.43              |
| 10:C32:144:ASP:CB   | 10:C32:147:LEU:HD12 | 2.44                     | 0.43              |
| 10:C32:736:ILE:HD11 | 10:C32:794:LYS:NZ   | 2.34                     | 0.43              |
| 10:C32:1082:ILE:O   | 10:C32:1084:LYS:N   | 2.51                     | 0.43              |
| 12:A48:629:LEU:HD22 | 12:A48:675:LEU:HD12 | 2.00                     | 0.43              |
| 1:R:1369:LEU:HD13   | 6:O:211:ASN:OD1     | 2.18                     | 0.43              |
| 2:M:239:LEU:HG      | 2:M:297:VAL:HG11    | 2.00                     | 0.43              |
| 2:M:307:PHE:O       | 2:M:311:GLN:HG2     | 2.18                     | 0.43              |
| 1:R8:526:ASN:O      | 1:R8:529:HIS:CE1    | 2.71                     | 0.43              |
| 1:R16:1449:TRP:HH2  | 2:M16:161:ASP:N     | 2.17                     | 0.43              |
| 2:M16:816:ARG:HH22  | 2:M16:849:LEU:HB3   | 1.83                     | 0.43              |
| 2:M16:847:PHE:CE1   | 4:T16:656:TRP:HB3   | 1.98                     | 0.43              |
| 5:P:68:GLY:HA3      | 6:O:9:ASP:O         | 2.18                     | 0.43              |
| 6:O:294:THR:OG1     | 6:O:308:GLN:NE2     | 2.31                     | 0.43              |
| 7:Q:22:VAL:HG12     | 7:Q:335:SER:OG      | 2.19                     | 0.43              |
| 5:P8:101:LEU:HD22   | 5:P8:133:TYR:CD2    | 2.51                     | 0.43              |
| 5:P8:214:LEU:CD2    | 5:P8:236:VAL:HG12   | 2.45                     | 0.43              |
| 5:P8:402:LEU:HD11   | 5:P8:433:LEU:HB3    | 2.00                     | 0.43              |
| 5:P8:614:VAL:CA     | 5:P8:629:ARG:NH2    | 2.81                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 7:Q8:149:VAL:CG2     | 7:Q8:187:TRP:CE2     | 2.99                     | 0.43              |
| 7:Q16:22:VAL:HG12    | 7:Q16:335:SER:OG     | 2.19                     | 0.43              |
| 8:L8:608:PHE:CZ      | 8:L8:635:MET:O       | 2.69                     | 0.43              |
| 9:K:587:LEU:HD23     | 9:K:608:LEU:HD23     | 2.00                     | 0.43              |
| 9:K:1048:GLN:OE1     | 9:K:1128:ARG:CD      | 2.66                     | 0.43              |
| 9:K8:1259:LYS:HE3    | 9:K8:1284:MET:HE3    | 1.33                     | 0.43              |
| 11:A24:257:GLN:HG2   | 11:A24:263:ASP:CG    | 2.43                     | 0.43              |
| 10:C24:182:ASP:CB    | 10:C24:183:PRO:HD2   | 2.31                     | 0.43              |
| 10:C24:196:ILE:CG2   | 10:C24:200:GLY:HA2   | 2.48                     | 0.43              |
| 10:C24:573:GLU:OE1   | 10:C24:617:TYR:OH    | 2.32                     | 0.43              |
| 10:C24:1085:SER:HB3  | 10:C24:1088:LEU:HD12 | 2.00                     | 0.43              |
| 10:C24:1488:ILE:O    | 10:C24:1494:ILE:HD12 | 2.18                     | 0.43              |
| 10:C24:1623:ILE:HG22 | 10:C24:1623:ILE:O    | 2.18                     | 0.43              |
| 10:C24:1767:LEU:CD1  | 10:C24:1832:MET:CE   | 2.96                     | 0.43              |
| 10:C24:1823:GLN:O    | 10:C24:1827:THR:OG1  | 2.33                     | 0.43              |
| 11:A40:375:ALA:N     | 11:A40:376:PRO:CD    | 2.81                     | 0.43              |
| 12:A:464:GLY:C       | 12:A:466:SER:N       | 2.74                     | 0.43              |
| 12:A:762:ILE:CD1     | 12:A:781:LEU:HD11    | 2.48                     | 0.43              |
| 12:A:785:HIS:CG      | 12:A:793:ALA:HB2     | 2.54                     | 0.43              |
| 10:C:179:ASN:OD1     | 10:C:213:ARG:NH1     | 2.52                     | 0.43              |
| 10:C:1002:LEU:HD23   | 10:C:1012:ARG:NH2    | 2.31                     | 0.43              |
| 10:C8:750:TYR:OH     | 10:C8:819:GLN:OE1    | 2.33                     | 0.43              |
| 10:C8:1157:LEU:HD22  | 10:C8:1176:VAL:HG11  | 2.01                     | 0.43              |
| 10:C8:1619:PRO:HB2   | 10:C8:1621:LYS:HG3   | 2.01                     | 0.43              |
| 17:F16:73:GLY:C      | 17:F16:75:ALA:N      | 2.76                     | 0.43              |
| 18:B:1859:LEU:HB3    | 18:B:1860:PRO:HD2    | 2.00                     | 0.43              |
| 18:B8:437:PHE:CZ     | 18:B8:473:LEU:HD13   | 2.54                     | 0.43              |
| 18:B8:484:TYR:CD2    | 18:B8:556:ILE:CD1    | 3.01                     | 0.43              |
| 18:B8:1496:GLY:HA3   | 24:D32:1302:ASP:OD2  | 2.18                     | 0.43              |
| 18:B8:1900:ILE:CD1   | 18:B8:1946:LEU:CD2   | 2.77                     | 0.43              |
| 20:E:261:PRO:HB3     | 20:E:297:TRP:HZ3     | 1.83                     | 0.43              |
| 20:E:381:SER:O       | 20:E:385:ASP:HB3     | 2.17                     | 0.43              |
| 19:48:97:LEU:HD21    | 19:48:232:TYR:CD1    | 2.52                     | 0.43              |
| 20:E8:261:PRO:HB3    | 20:E8:297:TRP:HZ3    | 1.83                     | 0.43              |
| 21:H:319:GLY:O       | 21:H:321:SER:N       | 2.51                     | 0.43              |
| 22:I:199:PHE:HB3     | 23:J32:620:MET:CE    | 2.48                     | 0.43              |
| 22:I:203:GLN:NE2     | 22:I:209:TRP:HE1     | 2.16                     | 0.43              |
| 21:H8:373:MET:HE2    | 22:I8:343:ARG:NH1    | 2.32                     | 0.43              |
| 22:I24:146:SER:HA    | 23:J24:571:TRP:CZ2   | 2.53                     | 0.43              |
| 22:I24:199:PHE:HB3   | 23:J24:620:MET:CE    | 2.48                     | 0.43              |
| 24:D:307:GLY:C       | 24:D16:753:ARG:NH2   | 2.67                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D40:1292:LYS:CE   | 24:D40:1337:ALA:HA   | 2.48                     | 0.43              |
| 10:C32:57:VAL:HG22   | 10:C32:62:ILE:CD1    | 2.47                     | 0.43              |
| 10:C32:445:MET:HE1   | 10:C32:462:PHE:CE1   | 2.52                     | 0.43              |
| 10:C32:630:SER:C     | 10:C32:632:GLN:H     | 2.27                     | 0.43              |
| 10:C32:1085:SER:HB3  | 10:C32:1088:LEU:HD12 | 2.01                     | 0.43              |
| 10:C32:1277:SER:HG   | 10:C32:1279:THR:HG1  | 1.64                     | 0.43              |
| 1:R:1132:TYR:OH      | 1:R:1214:ILE:HD13    | 2.19                     | 0.43              |
| 2:M:421:LEU:CD1      | 8:L:346:TRP:HE1      | 2.31                     | 0.43              |
| 3:N:19:MET:HG2       | 3:N:23:GLY:HA2       | 2.00                     | 0.43              |
| 1:R8:1124:TRP:CH2    | 4:T8:669:PRO:CG      | 2.96                     | 0.43              |
| 1:R8:1424:LYS:O      | 1:R8:1428:VAL:HG23   | 2.18                     | 0.43              |
| 2:M8:458:LYS:HE2     | 2:M8:472:GLN:CD      | 2.43                     | 0.43              |
| 2:M16:458:LYS:HE2    | 2:M16:472:GLN:CD     | 2.43                     | 0.43              |
| 2:M16:572:HIS:CG     | 2:M16:573:MET:N      | 2.86                     | 0.43              |
| 3:N16:97:HIS:HD2     | 3:N16:99:PHE:CZ      | 2.36                     | 0.43              |
| 5:P:247:GLU:OE1      | 5:P:295:LYS:CA       | 2.66                     | 0.43              |
| 7:Q8:22:VAL:HG12     | 7:Q8:335:SER:OG      | 2.19                     | 0.43              |
| 8:L16:851:PRO:HB2    | 9:K16:1283:PRO:CB    | 2.41                     | 0.43              |
| 9:K:919:MET:HG3      | 9:K:920:GLU:N        | 2.33                     | 0.43              |
| 9:K8:577:GLN:CD      | 9:K8:625:ARG:NH1     | 2.76                     | 0.43              |
| 9:K8:1133:ILE:CG2    | 9:K8:1166:LEU:CD2    | 2.97                     | 0.43              |
| 10:C16:1050:HIS:CD2  | 10:C16:1086:LYS:HZ1  | 1.97                     | 0.43              |
| 10:C16:1257:ALA:C    | 10:C16:1323:LEU:HD11 | 2.43                     | 0.43              |
| 10:C16:1352:GLN:NE2  | 10:C16:1357:LEU:HD12 | 2.33                     | 0.43              |
| 10:C16:1477:GLN:HG2  | 24:D8:1407:PHE:HB3   | 2.01                     | 0.43              |
| 10:C16:1594:PRO:HG3  | 10:C16:1642:TYR:CD2  | 2.54                     | 0.43              |
| 10:C16:1821:VAL:HB   | 11:A24:144:LYS:NZ    | 2.32                     | 0.43              |
| 11:A24:103:GLU:CD    | 21:H8:323:TYR:CZ     | 2.97                     | 0.43              |
| 11:A24:468:VAL:CG1   | 24:D16:1100:GLN:HB3  | 2.47                     | 0.43              |
| 10:C24:456:ASN:C     | 10:C24:458:VAL:N     | 2.76                     | 0.43              |
| 10:C24:764:ILE:HD13  | 10:C24:781:VAL:HG21  | 1.94                     | 0.43              |
| 10:C24:1069:TYR:HA   | 10:C24:1070:PRO:HD3  | 1.65                     | 0.43              |
| 10:C24:1449:GLU:OE1  | 24:D24:1151:SER:CB   | 2.65                     | 0.43              |
| 10:C24:1453:ARG:HH12 | 24:D24:1150:GLY:HA3  | 1.79                     | 0.43              |
| 10:C24:1477:GLN:HG2  | 24:D24:1407:PHE:CB   | 2.48                     | 0.43              |
| 10:C24:1594:PRO:HG3  | 10:C24:1642:TYR:CD2  | 2.54                     | 0.43              |
| 11:A40:257:GLN:HG2   | 11:A40:263:ASP:CG    | 2.43                     | 0.43              |
| 13:V:925:ILE:HD11    | 14:W:801:ALA:HB3     | 1.96                     | 0.43              |
| 14:W:705:HIS:HB3     | 15:J:644:ARG:NH1     | 2.33                     | 0.43              |
| 10:C:280:SER:C       | 10:C:282:LYS:N       | 2.74                     | 0.43              |
| 10:C:368:VAL:O       | 10:C:371:THR:OG1     | 2.36                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:722:LEU:HA      | 10:C:725:LEU:HD12    | 2.00                     | 0.43              |
| 10:C:1109:VAL:O      | 10:C:1111:SER:N      | 2.51                     | 0.43              |
| 10:C:1215:ALA:HA     | 10:C:1219:ILE:HD12   | 1.99                     | 0.43              |
| 10:C:1488:ILE:HD13   | 10:C:1528:LEU:HD23   | 1.99                     | 0.43              |
| 10:C8:105:TRP:O      | 10:C8:106:GLY:O      | 2.36                     | 0.43              |
| 10:C8:510:TRP:HB2    | 10:C8:511:PRO:HD3    | 2.01                     | 0.43              |
| 10:C8:605:GLU:H      | 10:C8:605:GLU:HG2    | 1.47                     | 0.43              |
| 11:A16:762:ILE:CD1   | 11:A16:781:LEU:HD11  | 2.48                     | 0.43              |
| 11:A16:763:HIS:ND1   | 11:A16:815:VAL:HG21  | 2.33                     | 0.43              |
| 11:A32:762:ILE:CD1   | 11:A32:781:LEU:HD11  | 2.48                     | 0.43              |
| 11:A32:763:HIS:ND1   | 11:A32:815:VAL:HG21  | 2.33                     | 0.43              |
| 18:B:313:ILE:CD1     | 18:B:331:TRP:CE3     | 3.02                     | 0.43              |
| 18:B:1658:MET:HE3    | 18:B:1658:MET:HB3    | 1.90                     | 0.43              |
| 18:B8:7:VAL:HG21     | 18:B8:99:ILE:CD1     | 2.48                     | 0.43              |
| 18:B8:65:LEU:CD1     | 18:B8:98:GLU:HB3     | 2.49                     | 0.43              |
| 18:B8:1349:LEU:HD22  | 18:B8:1367:ILE:CD1   | 2.46                     | 0.43              |
| 20:E:342:GLN:HB3     | 20:E:343:THR:H       | 1.74                     | 0.43              |
| 20:E:408:LEU:HD12    | 20:E:507:LEU:HD23    | 2.01                     | 0.43              |
| 19:48:175:TYR:CZ     | 20:E8:518:GLN:HG2    | 2.54                     | 0.43              |
| 20:E8:33:PHE:CD1     | 20:E8:37:LEU:HD12    | 2.46                     | 0.43              |
| 20:E8:353:ILE:CB     | 20:E8:413:PHE:CD2    | 3.01                     | 0.43              |
| 20:E8:494:ILE:HD13   | 20:E8:507:LEU:CB     | 2.47                     | 0.43              |
| 21:H24:319:GLY:O     | 21:H24:321:SER:N     | 2.51                     | 0.43              |
| 22:I16:203:GLN:O     | 22:I16:209:TRP:CE3   | 2.72                     | 0.43              |
| 24:D24:1170:VAL:HG22 | 24:D24:1232:VAL:HG22 | 2.01                     | 0.43              |
| 10:C32:102:ASN:HA    | 10:C32:107:LEU:HG    | 2.00                     | 0.43              |
| 10:C32:179:ASN:OD1   | 10:C32:213:ARG:NH1   | 2.52                     | 0.43              |
| 10:C32:300:VAL:HG12  | 10:C32:317:ARG:HG2   | 1.99                     | 0.43              |
| 10:C32:1109:VAL:C    | 10:C32:1111:SER:H    | 2.27                     | 0.43              |
| 10:C32:1457:LEU:HD23 | 10:C32:1521:ILE:HD13 | 2.00                     | 0.43              |
| 10:C32:1686:LEU:CD2  | 10:C32:1810:LEU:CD2  | 2.94                     | 0.43              |
| 1:R:1290:ILE:HD13    | 10:C:605:GLU:OE1     | 2.18                     | 0.43              |
| 2:M:572:HIS:CG       | 2:M:573:MET:N        | 2.86                     | 0.43              |
| 1:R8:1437:VAL:HG12   | 1:R8:1438:TRP:N      | 2.33                     | 0.43              |
| 1:R8:1444:VAL:HG11   | 1:R8:1475:LEU:HD11   | 2.01                     | 0.43              |
| 1:R16:684:ASP:CG     | 1:R16:784:TRP:HE1    | 2.26                     | 0.43              |
| 1:R16:746:GLU:CD     | 1:R16:835:ARG:HE     | 2.25                     | 0.43              |
| 2:M16:339:GLU:OE2    | 4:T8:639:ASP:OD1     | 2.35                     | 0.43              |
| 2:M16:625:HIS:NE2    | 3:N16:225:PRO:HB3    | 2.34                     | 0.43              |
| 5:P8:645:LEU:N       | 5:P8:646:PRO:CD      | 2.82                     | 0.43              |
| 7:Q8:231:HIS:NE2     | 7:Q8:283:GLU:OE2     | 2.40                     | 0.43              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 7:Q8:297:VAL:HG13    | 7:Q8:301:ARG:CB     | 2.44                     | 0.43              |
| 7:Q16:219:GLY:CA     | 7:Q16:221:TRP:CD1   | 3.01                     | 0.43              |
| 7:Q16:279:LEU:HD13   | 7:Q16:323:PRO:HB2   | 1.99                     | 0.43              |
| 8:L:601:HIS:ND1      | 8:L:631:LEU:HD22    | 2.08                     | 0.43              |
| 9:K:916:LYS:CB       | 9:K:919:MET:HE2     | 2.42                     | 0.43              |
| 9:K:1085:TYR:CD1     | 9:K:1097:VAL:HG23   | 2.53                     | 0.43              |
| 10:C16:296:PHE:CE1   | 10:C16:300:VAL:CG2  | 3.00                     | 0.43              |
| 11:A24:629:LEU:HD22  | 11:A24:675:LEU:HD12 | 2.01                     | 0.43              |
| 10:C24:296:PHE:CE1   | 10:C24:300:VAL:CG2  | 3.00                     | 0.43              |
| 10:C24:736:ILE:HD11  | 10:C24:794:LYS:NZ   | 2.33                     | 0.43              |
| 10:C24:1059:ALA:O    | 10:C24:1061:ASN:N   | 2.52                     | 0.43              |
| 10:C24:1420:LEU:HD22 | 10:C24:1471:TYR:CE2 | 2.52                     | 0.43              |
| 10:C24:1449:GLU:OE1  | 24:D24:1151:SER:CA  | 2.67                     | 0.43              |
| 11:A40:628:LEU:HG    | 11:A40:637:LEU:HD12 | 2.00                     | 0.43              |
| 14:W:210:PRO:HB3     | 14:W:219:ILE:HD11   | 1.99                     | 0.43              |
| 14:W:705:HIS:CB      | 15:J:644:ARG:NH1    | 2.81                     | 0.43              |
| 14:W:705:HIS:C       | 14:W:707:LYS:H      | 2.27                     | 0.43              |
| 10:C:1619:PRO:HB2    | 10:C:1621:LYS:HG3   | 2.00                     | 0.43              |
| 10:C8:547:VAL:HG21   | 10:C8:587:TYR:CD2   | 2.52                     | 0.43              |
| 10:C8:1109:VAL:C     | 10:C8:1111:SER:H    | 2.26                     | 0.43              |
| 10:C8:1626:GLN:HE21  | 10:C8:1692:LYS:CE   | 2.31                     | 0.43              |
| 10:C8:1686:LEU:CD2   | 10:C8:1810:LEU:CD2  | 2.94                     | 0.43              |
| 10:C8:1708:ARG:CA    | 10:C8:1730:ILE:HD11 | 2.48                     | 0.43              |
| 10:C8:1767:LEU:CD1   | 10:C8:1832:MET:CE   | 2.96                     | 0.43              |
| 11:A16:676:TYR:CD2   | 24:D16:1395:SER:HB2 | 2.48                     | 0.43              |
| 11:A16:798:PHE:CE2   | 11:A16:809:VAL:HG21 | 2.52                     | 0.43              |
| 11:A32:375:ALA:N     | 11:A32:376:PRO:CD   | 2.81                     | 0.43              |
| 18:B:268:GLN:HE21    | 18:B:323:GLU:HB3    | 1.76                     | 0.43              |
| 18:B:484:TYR:CD2     | 18:B:556:ILE:CD1    | 3.01                     | 0.43              |
| 18:B:957:ALA:CA      | 18:B:964:LEU:HD22   | 2.49                     | 0.43              |
| 18:B:1112:LYS:CE     | 21:H:327:SER:HA     | 2.33                     | 0.43              |
| 18:B:1649:SER:CA     | 18:B:1653:LEU:HD12  | 2.44                     | 0.43              |
| 18:B8:772:LYS:HE2    | 18:B8:839:ASP:HB3   | 1.99                     | 0.43              |
| 18:B8:1415:LEU:CD1   | 18:B8:1461:VAL:HG13 | 2.48                     | 0.43              |
| 20:E:449:ARG:C       | 20:E:452:GLY:H      | 2.26                     | 0.43              |
| 20:E8:342:GLN:HB3    | 20:E8:343:THR:H     | 1.74                     | 0.43              |
| 22:I:146:SER:HA      | 23:J32:571:TRP:CZ2  | 2.53                     | 0.43              |
| 24:D:308:ASN:HD21    | 24:D16:753:ARG:CG   | 2.31                     | 0.43              |
| 24:D:405:GLN:CD      | 24:D16:10:ARG:HE    | 2.04                     | 0.43              |
| 24:D:1292:LYS:CE     | 24:D:1337:ALA:HA    | 2.48                     | 0.43              |
| 24:D8:973:LEU:HD21   | 24:D8:977:LYS:HE3   | 2.01                     | 0.43              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 24:D8:1170:VAL:HG22 | 24:D8:1232:VAL:HG22  | 2.01                     | 0.43              |
| 24:D16:973:LEU:HD21 | 24:D16:977:LYS:HE3   | 2.01                     | 0.43              |
| 24:D24:7:ILE:HD12   | 24:D24:878:SER:CB    | 2.49                     | 0.43              |
| 10:C32:1442:GLN:O   | 10:C32:1444:GLY:N    | 2.50                     | 0.43              |
| 1:R:768:LEU:HG      | 24:D:1362:VAL:HA     | 2.00                     | 0.43              |
| 1:R:1490:VAL:O      | 1:R:1494:THR:OG1     | 2.36                     | 0.43              |
| 2:M:351:ALA:O       | 2:M:353:ILE:N        | 2.51                     | 0.43              |
| 1:R8:422:ARG:HH22   | 1:R8:584:GLY:CA      | 2.32                     | 0.43              |
| 1:R8:1124:TRP:CE3   | 1:R8:1170:LEU:C      | 2.97                     | 0.43              |
| 2:M8:339:GLU:C      | 2:M8:341:ASP:N       | 2.76                     | 0.43              |
| 3:N8:200:MET:CE     | 3:N8:203:PHE:CD2     | 2.96                     | 0.43              |
| 1:R16:1124:TRP:CE3  | 1:R16:1170:LEU:C     | 2.97                     | 0.43              |
| 1:R16:1437:VAL:HG12 | 1:R16:1438:TRP:N     | 2.33                     | 0.43              |
| 2:M16:157:GLY:HA3   | 3:N16:7:GLU:CD       | 2.44                     | 0.43              |
| 8:L8:1092:LEU:HD22  | 9:K8:999:PHE:CD2     | 2.53                     | 0.43              |
| 10:C16:105:TRP:O    | 10:C16:106:GLY:O     | 2.36                     | 0.43              |
| 10:C16:280:SER:C    | 10:C16:282:LYS:N     | 2.74                     | 0.43              |
| 10:C16:1121:ILE:O   | 10:C16:1133:ILE:HD12 | 2.19                     | 0.43              |
| 10:C16:1547:LYS:CD  | 24:D8:1406:SER:CB    | 2.96                     | 0.43              |
| 11:A24:375:ALA:N    | 11:A24:376:PRO:CD    | 2.81                     | 0.43              |
| 10:C24:102:ASN:HA   | 10:C24:107:LEU:HG    | 2.00                     | 0.43              |
| 10:C24:453:LEU:CG   | 10:C24:486:LEU:HD21  | 2.48                     | 0.43              |
| 10:C24:547:VAL:HG21 | 10:C24:587:TYR:CD2   | 2.52                     | 0.43              |
| 10:C24:630:SER:C    | 10:C24:632:GLN:H     | 2.27                     | 0.43              |
| 11:A40:763:HIS:ND1  | 11:A40:815:VAL:HG21  | 2.33                     | 0.43              |
| 11:A40:785:HIS:CG   | 11:A40:793:ALA:HB2   | 2.54                     | 0.43              |
| 12:A:375:ALA:N      | 12:A:376:PRO:CD      | 2.81                     | 0.43              |
| 13:V:825:GLN:O      | 14:W:707:LYS:NZ      | 2.51                     | 0.43              |
| 14:W:638:VAL:CG2    | 15:J:561:PHE:HZ      | 2.30                     | 0.43              |
| 10:C:1163:LEU:HB3   | 10:C:1166:SER:OG     | 2.19                     | 0.43              |
| 10:C:1507:LEU:C     | 10:C:1509:SER:N      | 2.67                     | 0.43              |
| 10:C:1725:THR:C     | 10:C:1727:SER:N      | 2.76                     | 0.43              |
| 10:C8:1385:LEU:HD23 | 10:C8:1389:ILE:CD1   | 2.47                     | 0.43              |
| 10:C8:1725:THR:C    | 10:C8:1727:SER:N     | 2.77                     | 0.43              |
| 11:A16:794:THR:C    | 11:A16:796:ASP:N     | 2.77                     | 0.43              |
| 11:A32:794:THR:C    | 11:A32:796:ASP:N     | 2.77                     | 0.43              |
| 18:B:154:LEU:CD2    | 18:B:224:GLU:OE1     | 2.67                     | 0.43              |
| 18:B:154:LEU:HD22   | 18:B:224:GLU:OE1     | 2.19                     | 0.43              |
| 18:B:176:GLU:OE1    | 18:B:222:TYR:OH      | 2.34                     | 0.43              |
| 18:B:410:GLN:HG3    | 18:B:538:ARG:HH22    | 1.82                     | 0.43              |
| 18:B:495:THR:CG2    | 18:B:549:TRP:CD1     | 3.02                     | 0.43              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B:1960:LEU:HD23  | 18:B:1961:TYR:CE2    | 2.53                     | 0.43              |
| 18:B8:49:GLY:O      | 18:B8:52:SER:OG      | 2.27                     | 0.43              |
| 18:B8:154:LEU:CD2   | 18:B8:224:GLU:OE1    | 2.67                     | 0.43              |
| 18:B8:957:ALA:CA    | 18:B8:964:LEU:HD22   | 2.49                     | 0.43              |
| 18:B8:1662:TYR:CZ   | 18:B8:1692:VAL:HG11  | 2.53                     | 0.43              |
| 19:4:97:LEU:HD21    | 19:4:232:TYR:CD1     | 2.52                     | 0.43              |
| 19:4:125:ILE:CD1    | 19:4:139:LEU:HD11    | 2.49                     | 0.43              |
| 20:E:123:CYS:SG     | 20:E:135:ILE:CG2     | 2.99                     | 0.43              |
| 20:E:429:PRO:HB2    | 20:E:430:ALA:H       | 1.67                     | 0.43              |
| 19:48:244:GLN:NE2   | 20:E8:364:PHE:CE1    | 2.87                     | 0.43              |
| 20:E8:350:GLU:CG    | 20:E8:352:PHE:HE2    | 2.30                     | 0.43              |
| 20:E8:480:MET:HE3   | 20:E8:493:TRP:CZ3    | 2.53                     | 0.43              |
| 22:I:300:LEU:CG     | 23:J32:689:LEU:HD21  | 2.41                     | 0.43              |
| 22:I8:332:MET:HG3   | 23:J8:732:MET:HE1    | 2.00                     | 0.43              |
| 21:H24:267:LYS:HZ2  | 23:J24:631:GLU:HB3   | 1.84                     | 0.43              |
| 22:I24:203:GLN:O    | 22:I24:209:TRP:CE3   | 2.72                     | 0.43              |
| 22:I16:332:MET:HG3  | 23:J16:732:MET:HE1   | 2.00                     | 0.43              |
| 24:D:1170:VAL:HG22  | 24:D:1232:VAL:HG22   | 2.01                     | 0.43              |
| 24:D16:7:ILE:HD12   | 24:D16:878:SER:CB    | 2.49                     | 0.43              |
| 24:D24:1292:LYS:CE  | 24:D24:1337:ALA:HA   | 2.48                     | 0.43              |
| 24:D40:472:ILE:HD11 | 24:D40:539:THR:CG2   | 2.48                     | 0.43              |
| 10:C32:57:VAL:HG22  | 10:C32:62:ILE:HD11   | 2.01                     | 0.43              |
| 10:C32:182:ASP:OD1  | 10:C32:182:ASP:N     | 2.52                     | 0.43              |
| 10:C32:448:LYS:O    | 10:C32:450:PRO:CD    | 2.57                     | 0.43              |
| 10:C32:1352:GLN:NE2 | 10:C32:1357:LEU:HD12 | 2.32                     | 0.43              |
| 10:C32:1770:LEU:O   | 10:C32:1836:LYS:NZ   | 2.51                     | 0.43              |
| 12:A48:798:PHE:CE2  | 12:A48:809:VAL:HG21  | 2.52                     | 0.43              |
| 1:R:1424:LYS:O      | 1:R:1428:VAL:HG23    | 2.18                     | 0.43              |
| 1:R:1444:VAL:HG11   | 1:R:1475:LEU:HD11    | 2.01                     | 0.43              |
| 2:M:217:ILE:HD11    | 3:N:28:THR:CG2       | 2.42                     | 0.43              |
| 2:M:339:GLU:C       | 2:M:341:ASP:N        | 2.76                     | 0.43              |
| 2:M8:417:ARG:CG     | 8:L8:298:PHE:CD2     | 3.02                     | 0.43              |
| 3:N8:158:TRP:CZ2    | 3:N8:179:LEU:HD21    | 2.48                     | 0.43              |
| 1:R16:1124:TRP:HZ2  | 4:T16:669:PRO:HD3    | 1.83                     | 0.43              |
| 3:N16:4:GLN:CD      | 3:N16:44:GLY:HA2     | 2.40                     | 0.43              |
| 5:P:566:PHE:CZ      | 5:P:597:GLY:O        | 2.71                     | 0.43              |
| 7:Q8:222:PHE:O      | 7:Q8:223:GLN:C       | 2.62                     | 0.43              |
| 9:K:584:SER:C       | 9:K:622:VAL:HG11     | 2.44                     | 0.43              |
| 9:K:646:ILE:HA      | 9:K:649:MET:CE       | 2.49                     | 0.43              |
| 9:K:840:TRP:CZ3     | 9:K:907:ILE:HG13     | 2.54                     | 0.43              |
| 9:K:1069:PRO:O      | 9:K:1126:LEU:HD12    | 2.18                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:K8:714:ARG:NH1     | 9:K8:731:CYS:SG      | 2.91                     | 0.43              |
| 9:K8:842:ILE:HG23    | 9:K8:871:LEU:CD2     | 2.48                     | 0.43              |
| 10:C16:510:TRP:HB2   | 10:C16:511:PRO:HD3   | 2.00                     | 0.43              |
| 10:C16:736:ILE:HD11  | 10:C16:794:LYS:NZ    | 2.33                     | 0.43              |
| 10:C16:768:ARG:HD3   | 10:C16:778:GLU:HB2   | 2.01                     | 0.43              |
| 10:C16:1109:VAL:O    | 10:C16:1111:SER:N    | 2.51                     | 0.43              |
| 10:C16:1109:VAL:C    | 10:C16:1111:SER:H    | 2.27                     | 0.43              |
| 10:C16:1297:HIS:CE1  | 10:C16:1372:ALA:HB1  | 2.54                     | 0.43              |
| 11:A24:103:GLU:OE1   | 21:H8:323:TYR:CE2    | 2.72                     | 0.43              |
| 10:C24:1442:GLN:O    | 10:C24:1444:GLY:N    | 2.49                     | 0.43              |
| 10:C24:1725:THR:C    | 10:C24:1727:SER:H    | 2.26                     | 0.43              |
| 13:V:910:GLU:N       | 14:W:787:MET:CE      | 2.82                     | 0.43              |
| 10:C:1624:LEU:CD2    | 10:C:1632:LEU:CD1    | 2.96                     | 0.43              |
| 10:C:1823:GLN:O      | 10:C:1827:THR:OG1    | 2.33                     | 0.43              |
| 10:C8:1328:PHE:CZ    | 10:C8:1377:ILE:CD1   | 2.92                     | 0.43              |
| 10:C8:1385:LEU:HD11  | 10:C8:1419:PHE:HD1   | 1.84                     | 0.43              |
| 11:A32:587:VAL:HG21  | 11:A32:636:PHE:CE1   | 2.41                     | 0.43              |
| 18:B:538:ARG:O       | 18:B:545:VAL:HG13    | 2.18                     | 0.43              |
| 18:B:583:ARG:HH11    | 18:B:643:MET:HE1     | 1.79                     | 0.43              |
| 18:B:1209:LEU:HD23   | 18:B:1238:PHE:HE1    | 1.84                     | 0.43              |
| 18:B:1490:ILE:O      | 18:B:1494:THR:HG23   | 2.19                     | 0.43              |
| 18:B:1697:LEU:HD11   | 18:B:1826:VAL:HG13   | 2.01                     | 0.43              |
| 18:B8:86:LYS:CE      | 18:B8:123:LEU:HD11   | 2.48                     | 0.43              |
| 18:B8:135:TYR:OH     | 18:B8:139:ARG:NH1    | 2.48                     | 0.43              |
| 18:B8:410:GLN:HG3    | 18:B8:538:ARG:HH22   | 1.82                     | 0.43              |
| 18:B8:603:PHE:HB3    | 18:B8:619:ARG:NH2    | 2.29                     | 0.43              |
| 18:B8:1194:LEU:HD11  | 18:B8:1311:TRP:CH2   | 2.52                     | 0.43              |
| 18:B8:1438:LEU:CD1   | 18:B8:1462:LEU:HD11  | 2.49                     | 0.43              |
| 18:B8:1490:ILE:O     | 18:B8:1494:THR:HG23  | 2.19                     | 0.43              |
| 20:E:480:MET:CE      | 20:E:493:TRP:CZ3     | 3.02                     | 0.43              |
| 23:J8:718:GLN:HG3    | 23:J8:737:TRP:CZ3    | 2.52                     | 0.43              |
| 24:D:212:GLU:HB2     | 24:D:230:LEU:HD11    | 2.01                     | 0.43              |
| 24:D24:973:LEU:HD21  | 24:D24:977:LYS:HE3   | 2.01                     | 0.43              |
| 24:D32:973:LEU:HD21  | 24:D32:977:LYS:HE3   | 2.01                     | 0.43              |
| 24:D40:973:LEU:HD21  | 24:D40:977:LYS:HE3   | 2.00                     | 0.43              |
| 24:D40:1380:LEU:HB3  | 24:D40:1454:LEU:HD21 | 2.00                     | 0.43              |
| 10:C32:453:LEU:CG    | 10:C32:486:LEU:HD21  | 2.48                     | 0.43              |
| 10:C32:918:PHE:HA    | 10:C32:927:THR:HG21  | 1.99                     | 0.43              |
| 10:C32:1157:LEU:HD22 | 10:C32:1176:VAL:HG11 | 2.01                     | 0.43              |
| 10:C32:1594:PRO:HG3  | 10:C32:1642:TYR:CD2  | 2.53                     | 0.43              |
| 12:A48:762:ILE:CD1   | 12:A48:781:LEU:HD11  | 2.48                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:R:1201:LEU:O      | 1:R:1202:ARG:C      | 2.56                     | 0.43              |
| 1:R:1330:ALA:CB     | 10:C:1173:LEU:HD13  | 2.45                     | 0.43              |
| 1:R8:1466:LYS:CG    | 6:O8:160:LEU:CD1    | 2.92                     | 0.43              |
| 2:M8:632:VAL:HG22   | 3:N8:222:LEU:HB3    | 2.01                     | 0.43              |
| 2:M16:762:LEU:HD22  | 2:M16:813:ASN:HD22  | 1.83                     | 0.43              |
| 5:P:1:MET:HA        | 5:P:2:PRO:HD3       | 1.50                     | 0.43              |
| 5:P:378:ASP:OD2     | 14:W:25:ARG:HD2     | 2.19                     | 0.43              |
| 7:Q:298:SER:C       | 7:Q:300:SER:N       | 2.75                     | 0.43              |
| 5:P8:281:ILE:HD11   | 5:P8:341:MET:CE     | 2.45                     | 0.43              |
| 5:P8:607:PHE:CE1    | 5:P8:611:LEU:HD13   | 2.54                     | 0.43              |
| 6:O8:133:LEU:HD11   | 6:O8:153:PHE:CE1    | 2.48                     | 0.43              |
| 7:Q8:136:ARG:NH1    | 7:Q8:138:GLU:CD     | 2.76                     | 0.43              |
| 5:P16:578:LEU:CD1   | 5:P16:608:LYS:HZ2   | 2.31                     | 0.43              |
| 9:K:751:LEU:HD23    | 9:K:754:ARG:HD3     | 1.98                     | 0.43              |
| 9:K:1133:ILE:CG2    | 9:K:1166:LEU:CD2    | 2.97                     | 0.43              |
| 9:K8:638:TRP:CH2    | 9:K8:754:ARG:HD2    | 2.54                     | 0.43              |
| 9:K8:700:MET:CE     | 9:K8:764:VAL:HA     | 2.48                     | 0.43              |
| 9:K8:840:TRP:HE3    | 9:K8:875:LEU:HD21   | 1.84                     | 0.43              |
| 10:C16:445:MET:HE1  | 10:C16:462:PHE:HZ   | 1.84                     | 0.43              |
| 10:C16:667:ILE:CG2  | 10:C16:670:GLU:O    | 2.67                     | 0.43              |
| 10:C16:1059:ALA:O   | 10:C16:1061:ASN:N   | 2.52                     | 0.43              |
| 11:A24:107:GLN:NE2  | 21:H8:324:LEU:O     | 2.42                     | 0.43              |
| 10:C24:47:PRO:HG2   | 10:C24:93:ASP:OD2   | 2.19                     | 0.43              |
| 10:C24:667:ILE:CG2  | 10:C24:670:GLU:O    | 2.67                     | 0.43              |
| 10:C24:761:VAL:HG21 | 10:C24:826:TYR:CA   | 2.42                     | 0.43              |
| 10:C24:855:VAL:N    | 10:C24:856:PRO:CD   | 2.82                     | 0.43              |
| 10:C24:1297:HIS:CE1 | 10:C24:1372:ALA:HB1 | 2.54                     | 0.43              |
| 10:C24:1567:LEU:HA  | 10:C24:1610:MET:HE1 | 2.00                     | 0.43              |
| 11:A40:24:ALA:O     | 23:J16:705:TRP:CZ2  | 2.70                     | 0.43              |
| 11:A40:66:LEU:CD1   | 22:I16:323:GLU:OE2  | 2.65                     | 0.43              |
| 11:A40:156:MET:N    | 11:A40:555:HIS:NE2  | 2.67                     | 0.43              |
| 14:W:750:HIS:O      | 14:W:753:THR:OG1    | 2.37                     | 0.43              |
| 10:C:1085:SER:HB3   | 10:C:1088:LEU:HD12  | 2.00                     | 0.43              |
| 10:C:1725:THR:C     | 10:C:1727:SER:H     | 2.26                     | 0.43              |
| 10:C8:64:LEU:CD1    | 10:C8:70:ILE:HD12   | 2.42                     | 0.43              |
| 10:C8:179:ASN:OD1   | 10:C8:213:ARG:NH1   | 2.52                     | 0.43              |
| 10:C8:1594:PRO:HG3  | 10:C8:1642:TYR:CD2  | 2.54                     | 0.43              |
| 11:A16:557:LEU:CD2  | 11:A16:561:ASP:CB   | 2.90                     | 0.43              |
| 11:A16:628:LEU:HG   | 11:A16:637:LEU:HD12 | 2.00                     | 0.43              |
| 11:A32:91:GLU:CD    | 18:B8:1112:LYS:HZ3  | 2.07                     | 0.43              |
| 11:A32:159:LYS:HZ2  | 18:B8:1918:ARG:CG   | 2.29                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:703:ALA:HA    | 24:D32:1398:ARG:HD2  | 1.92                     | 0.43              |
| 11:A32:703:ALA:CA    | 24:D32:1398:ARG:HH11 | 2.32                     | 0.43              |
| 18:B:83:LEU:HD22     | 18:B:105:VAL:HG12    | 2.00                     | 0.43              |
| 18:B:1660:SER:CA     | 18:B:1724:MET:HE1    | 2.49                     | 0.43              |
| 18:B8:495:THR:CG2    | 18:B8:549:TRP:CD1    | 3.02                     | 0.43              |
| 18:B8:1130:LEU:HD23  | 18:B8:1132:TRP:CD1   | 2.46                     | 0.43              |
| 18:B8:1234:MET:N     | 18:B8:1235:PRO:CD    | 2.81                     | 0.43              |
| 20:E8:306:SER:C      | 20:E8:308:GLU:N      | 2.76                     | 0.43              |
| 21:H8:322:LEU:CD1    | 23:J8:689:LEU:HG     | 2.46                     | 0.43              |
| 21:H16:319:GLY:O     | 21:H16:321:SER:N     | 2.51                     | 0.43              |
| 24:D8:7:ILE:HD12     | 24:D8:878:SER:CB     | 2.49                     | 0.43              |
| 24:D8:1284:ILE:HD11  | 24:D8:1319:ALA:HA    | 2.01                     | 0.43              |
| 24:D16:94:ALA:HB1    | 24:D16:543:MET:HE1   | 2.00                     | 0.43              |
| 24:D16:472:ILE:HD11  | 24:D16:539:THR:CG2   | 2.48                     | 0.43              |
| 24:D16:1284:ILE:HD11 | 24:D16:1319:ALA:HA   | 2.00                     | 0.43              |
| 10:C32:855:VAL:N     | 10:C32:856:PRO:CD    | 2.82                     | 0.43              |
| 12:A48:785:HIS:CG    | 12:A48:793:ALA:HB2   | 2.54                     | 0.43              |
| 1:R:1190:VAL:HG22    | 24:D:1456:GLU:C      | 2.44                     | 0.43              |
| 1:R:1360:GLN:C       | 10:C:608:ASP:OD2     | 2.62                     | 0.43              |
| 2:M:632:VAL:HG22     | 3:N:222:LEU:HB3      | 2.01                     | 0.43              |
| 2:M:732:TRP:CZ3      | 2:M:736:ALA:HB3      | 2.53                     | 0.43              |
| 3:N:278:ASP:OD1      | 3:N:278:ASP:C        | 2.62                     | 0.43              |
| 2:M8:572:HIS:CG      | 2:M8:573:MET:N       | 2.86                     | 0.43              |
| 2:M8:622:ARG:CZ      | 2:M8:624:ASP:OD2     | 2.64                     | 0.43              |
| 3:N8:221:ASN:C       | 3:N8:223:GLY:N       | 2.77                     | 0.43              |
| 1:R16:1269:LEU:CD1   | 5:P16:684:ARG:HD3    | 2.44                     | 0.43              |
| 3:N16:221:ASN:C      | 3:N16:223:GLY:N      | 2.77                     | 0.43              |
| 5:P:214:LEU:HD21     | 5:P:236:VAL:HG12     | 2.01                     | 0.43              |
| 5:P:398:LYS:HD2      | 5:P:426:MET:SD       | 2.59                     | 0.43              |
| 5:P:634:MET:HE3      | 5:P:674:LYS:HG3      | 2.01                     | 0.43              |
| 7:Q8:124:PHE:CE1     | 7:Q8:125:TYR:CE2     | 2.80                     | 0.43              |
| 7:Q8:149:VAL:HG22    | 7:Q8:159:VAL:HG22    | 2.01                     | 0.43              |
| 5:P16:47:ASN:ND2     | 5:P16:76:LEU:O       | 2.52                     | 0.43              |
| 5:P16:105:ARG:NH2    | 5:P16:133:TYR:CE1    | 2.66                     | 0.43              |
| 5:P16:115:MET:O      | 5:P16:119:SER:HB2    | 2.19                     | 0.43              |
| 5:P16:454:GLY:O      | 5:P16:488:LYS:NZ     | 2.51                     | 0.43              |
| 9:K:714:ARG:NH1      | 9:K:731:CYS:SG       | 2.92                     | 0.43              |
| 9:K8:1069:PRO:O      | 9:K8:1126:LEU:HD12   | 2.19                     | 0.43              |
| 9:K8:1085:TYR:CD1    | 9:K8:1097:VAL:HG23   | 2.53                     | 0.43              |
| 10:C16:41:GLN:NE2    | 10:C16:165:ALA:HB1   | 2.34                     | 0.43              |
| 10:C16:750:TYR:OH    | 10:C16:813:LEU:HD23  | 2.19                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:962:PHE:HZ    | 10:C16:997:ILE:CD1   | 2.18                     | 0.43              |
| 10:C16:1129:VAL:CG1  | 10:C16:1130:SER:N    | 2.81                     | 0.43              |
| 10:C16:1157:LEU:HD22 | 10:C16:1176:VAL:HG11 | 2.01                     | 0.43              |
| 10:C16:1282:CYS:HA   | 10:C16:1738:MET:CE   | 2.42                     | 0.43              |
| 10:C16:1626:GLN:HE21 | 10:C16:1692:LYS:CE   | 2.31                     | 0.43              |
| 11:A24:36:ASN:HD21   | 22:I8:293:LYS:HE3    | 1.76                     | 0.43              |
| 10:C24:182:ASP:OD1   | 10:C24:182:ASP:N     | 2.52                     | 0.43              |
| 10:C24:615:GLU:CA    | 10:C24:619:LEU:HD12  | 2.49                     | 0.43              |
| 10:C24:1449:GLU:OE2  | 24:D24:1151:SER:CB   | 2.67                     | 0.43              |
| 12:A:794:THR:C       | 12:A:796:ASP:N       | 2.77                     | 0.43              |
| 10:C:879:LEU:CD2     | 10:C:944:MET:HG3     | 2.49                     | 0.43              |
| 10:C8:736:ILE:HD11   | 10:C8:794:LYS:NZ     | 2.33                     | 0.43              |
| 10:C8:855:VAL:N      | 10:C8:856:PRO:CD     | 2.82                     | 0.43              |
| 11:A16:785:HIS:CG    | 11:A16:793:ALA:HB2   | 2.54                     | 0.43              |
| 11:A32:362:ARG:NE    | 11:A32:366:ARG:HH12  | 2.17                     | 0.43              |
| 18:B:65:LEU:CD1      | 18:B:98:GLU:HB3      | 2.49                     | 0.43              |
| 18:B:192:PRO:HG2     | 18:B:195:MET:SD      | 2.58                     | 0.43              |
| 18:B:690:TRP:CZ3     | 18:B:787:VAL:HG13    | 2.54                     | 0.43              |
| 18:B:1234:MET:N      | 18:B:1235:PRO:CD     | 2.81                     | 0.43              |
| 18:B8:1353:GLU:OE1   | 18:B8:1417:SER:OG    | 2.36                     | 0.43              |
| 18:B8:1697:LEU:HD11  | 18:B8:1826:VAL:HG13  | 2.01                     | 0.43              |
| 19:4:316:PHE:HB2     | 19:4:319:SER:HB3     | 2.01                     | 0.43              |
| 20:E:347:PRO:HA      | 20:E:348:PRO:HD3     | 1.76                     | 0.43              |
| 20:E:480:MET:HE3     | 20:E:493:TRP:CZ3     | 2.53                     | 0.43              |
| 20:E8:480:MET:CE     | 20:E8:493:TRP:CZ3    | 3.02                     | 0.43              |
| 21:H:231:HIS:CG      | 23:J32:596:GLN:HE22  | 2.31                     | 0.43              |
| 22:I:300:LEU:HD22    | 23:J32:689:LEU:CD2   | 2.42                     | 0.43              |
| 21:H24:271:LEU:HD21  | 22:I24:254:ILE:HG21  | 1.98                     | 0.43              |
| 21:H16:190:TRP:HA    | 21:H16:191:PRO:HD3   | 1.89                     | 0.43              |
| 21:H16:284:LEU:C     | 23:J16:650:GLN:NE2   | 2.77                     | 0.43              |
| 22:I16:199:PHE:HB3   | 23:J16:620:MET:CE    | 2.49                     | 0.43              |
| 24:D:1284:ILE:HD11   | 24:D:1319:ALA:HA     | 2.01                     | 0.43              |
| 24:D:1380:LEU:HB3    | 24:D:1454:LEU:HD21   | 2.00                     | 0.43              |
| 24:D16:1292:LYS:CE   | 24:D16:1337:ALA:HA   | 2.48                     | 0.43              |
| 24:D32:7:ILE:HD12    | 24:D32:878:SER:CB    | 2.49                     | 0.43              |
| 24:D40:1284:ILE:HD11 | 24:D40:1319:ALA:HA   | 2.00                     | 0.43              |
| 10:C32:41:GLN:NE2    | 10:C32:165:ALA:HB1   | 2.34                     | 0.43              |
| 10:C32:1105:LEU:HD21 | 10:C32:1183:LEU:HD21 | 2.01                     | 0.43              |
| 12:A48:642:GLY:O     | 12:A48:685:ARG:HD2   | 2.19                     | 0.43              |
| 2:M:641:CYS:HA       | 2:M:644:TRP:HE1      | 1.82                     | 0.42              |
| 3:N:1:MET:CB         | 3:N:302:PRO:O        | 2.57                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:730:GLU:HG3     | 8:L16:504:GLN:CG     | 2.49                     | 0.42              |
| 2:M8:847:PHE:CD1     | 4:T8:656:TRP:CE3     | 2.59                     | 0.42              |
| 7:Q:149:VAL:HG22     | 7:Q:159:VAL:HG22     | 2.01                     | 0.42              |
| 7:Q8:254:ALA:CB      | 7:Q8:302:ILE:CD1     | 2.97                     | 0.42              |
| 7:Q16:298:SER:C      | 7:Q16:300:SER:N      | 2.75                     | 0.42              |
| 9:K:584:SER:CB       | 9:K:622:VAL:HG21     | 2.42                     | 0.42              |
| 9:K:743:ARG:NH1      | 9:K:772:TYR:CD1      | 2.75                     | 0.42              |
| 9:K:745:ARG:HD2      | 9:K:752:MET:HA       | 2.00                     | 0.42              |
| 9:K:840:TRP:HE3      | 9:K:875:LEU:HD21     | 1.84                     | 0.42              |
| 9:K16:950:LYS:HE2    | 9:K16:974:LEU:HD21   | 1.99                     | 0.42              |
| 10:C16:919:ASP:H     | 10:C16:927:THR:HG23  | 1.84                     | 0.42              |
| 10:C16:1105:LEU:HD21 | 10:C16:1183:LEU:HD21 | 2.01                     | 0.42              |
| 10:C24:1105:LEU:HD21 | 10:C24:1183:LEU:HD21 | 2.01                     | 0.42              |
| 10:C24:1121:ILE:O    | 10:C24:1133:ILE:HD12 | 2.19                     | 0.42              |
| 10:C24:1129:VAL:CG1  | 10:C24:1130:SER:N    | 2.82                     | 0.42              |
| 14:W:646:ALA:N       | 14:W:647:PRO:CD      | 2.80                     | 0.42              |
| 10:C:553:LEU:CD2     | 10:C:595:THR:HG23    | 2.45                     | 0.42              |
| 10:C:630:SER:C       | 10:C:632:GLN:H       | 2.27                     | 0.42              |
| 10:C:667:ILE:CG2     | 10:C:670:GLU:O       | 2.67                     | 0.42              |
| 10:C:1623:ILE:HG22   | 10:C:1623:ILE:O      | 2.18                     | 0.42              |
| 10:C:1686:LEU:CD2    | 10:C:1810:LEU:CD2    | 2.94                     | 0.42              |
| 10:C8:1257:ALA:C     | 10:C8:1323:LEU:HD11  | 2.43                     | 0.42              |
| 10:C8:1763:LEU:HD13  | 10:C8:1825:LEU:HD23  | 2.00                     | 0.42              |
| 17:F:69:SER:HA       | 17:F:70:PRO:HD3      | 1.82                     | 0.42              |
| 11:A32:66:LEU:CD1    | 22:I24:323:GLU:OE2   | 2.65                     | 0.42              |
| 18:B:243:GLY:CA      | 18:B:248:SER:OG      | 2.67                     | 0.42              |
| 18:B:1375:SER:O      | 18:B:1379:VAL:HG23   | 2.19                     | 0.42              |
| 18:B:1601:VAL:HG12   | 18:B:1601:VAL:O      | 2.19                     | 0.42              |
| 18:B:1783:VAL:HG21   | 18:B:1810:VAL:HG21   | 2.01                     | 0.42              |
| 18:B:1900:ILE:CD1    | 18:B:1946:LEU:CD2    | 2.77                     | 0.42              |
| 18:B8:477:SER:HA     | 18:B8:588:PHE:O      | 2.19                     | 0.42              |
| 19:4:65:LYS:C        | 19:4:66:ALA:O        | 2.62                     | 0.42              |
| 19:4:94:VAL:O        | 19:4:97:LEU:HB2      | 2.18                     | 0.42              |
| 19:4:403:GLY:HA3     | 19:4:429:TRP:CE2     | 2.54                     | 0.42              |
| 20:E:31:PHE:CE1      | 20:E:46:PHE:HZ       | 2.36                     | 0.42              |
| 19:48:17:ARG:NH2     | 19:48:386:ASP:OD2    | 2.52                     | 0.42              |
| 19:48:269:PHE:HB3    | 19:48:281:TRP:HB2    | 2.01                     | 0.42              |
| 23:J32:733:ALA:HA    | 23:J32:734:PRO:HD3   | 1.47                     | 0.42              |
| 21:H8:284:LEU:C      | 23:J8:650:GLN:NE2    | 2.77                     | 0.42              |
| 23:J8:679:GLU:C      | 23:J8:681:GLU:H      | 2.27                     | 0.42              |
| 24:D8:1325:ARG:C     | 24:D8:1326:ILE:HG13  | 2.44                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:D32:1284:ILE:HD11 | 24:D32:1319:ALA:HA   | 2.00                     | 0.42              |
| 24:D40:873:ARG:HD2   | 24:D40:884:ASP:CB    | 2.49                     | 0.42              |
| 24:D40:1325:ARG:C    | 24:D40:1326:ILE:HG13 | 2.44                     | 0.42              |
| 10:C32:1129:VAL:CG1  | 10:C32:1130:SER:N    | 2.81                     | 0.42              |
| 10:C32:1265:ARG:HG2  | 10:C32:1268:ARG:HE   | 1.54                     | 0.42              |
| 10:C32:1725:THR:C    | 10:C32:1727:SER:H    | 2.26                     | 0.42              |
| 12:A48:504:TYR:HB3   | 12:A48:505:PRO:CD    | 2.46                     | 0.42              |
| 12:A48:849:TRP:HB2   | 12:A48:854:TYR:CE2   | 2.54                     | 0.42              |
| 1:R:422:ARG:HH22     | 1:R:584:GLY:CA       | 2.32                     | 0.42              |
| 1:R:1124:TRP:CE3     | 1:R:1170:LEU:C       | 2.97                     | 0.42              |
| 1:R:1154:LEU:HD13    | 1:R:1230:TYR:HA      | 2.00                     | 0.42              |
| 2:M:843:ALA:O        | 4:T:656:TRP:HH2      | 2.02                     | 0.42              |
| 3:N:169:SER:O        | 3:N:170:SER:C        | 2.62                     | 0.42              |
| 3:N16:278:ASP:OD1    | 3:N16:278:ASP:C      | 2.62                     | 0.42              |
| 5:P16:317:ILE:HG23   | 5:P16:342:LEU:HD22   | 2.00                     | 0.42              |
| 7:Q16:149:VAL:HG22   | 7:Q16:159:VAL:HG22   | 2.01                     | 0.42              |
| 9:K8:584:SER:C       | 9:K8:622:VAL:HG11    | 2.44                     | 0.42              |
| 10:C16:47:PRO:HG2    | 10:C16:93:ASP:OD2    | 2.19                     | 0.42              |
| 10:C16:102:ASN:HA    | 10:C16:107:LEU:HG    | 2.00                     | 0.42              |
| 10:C16:630:SER:C     | 10:C16:632:GLN:H     | 2.27                     | 0.42              |
| 10:C16:945:LEU:O     | 10:C16:993:HIS:HE1   | 2.03                     | 0.42              |
| 10:C16:1317:ARG:HD3  | 10:C16:1387:LEU:HD21 | 2.01                     | 0.42              |
| 10:C24:1109:VAL:C    | 10:C24:1111:SER:H    | 2.27                     | 0.42              |
| 14:W:515:CYS:O       | 14:W:607:ARG:HD2     | 2.19                     | 0.42              |
| 10:C:1297:HIS:CE1    | 10:C:1372:ALA:HB1    | 2.54                     | 0.42              |
| 10:C:1317:ARG:HD3    | 10:C:1387:LEU:HD21   | 2.01                     | 0.42              |
| 10:C:1708:ARG:CA     | 10:C:1730:ILE:HD11   | 2.48                     | 0.42              |
| 10:C8:47:PRO:HG2     | 10:C8:93:ASP:OD2     | 2.19                     | 0.42              |
| 10:C8:57:VAL:HG22    | 10:C8:62:ILE:HD11    | 2.01                     | 0.42              |
| 10:C8:508:ILE:HG23   | 10:C8:549:TYR:HH     | 1.83                     | 0.42              |
| 10:C8:750:TYR:OH     | 10:C8:813:LEU:HD23   | 2.19                     | 0.42              |
| 10:C8:1085:SER:HB3   | 10:C8:1088:LEU:HD12  | 2.00                     | 0.42              |
| 10:C8:1163:LEU:HB3   | 10:C8:1166:SER:OG    | 2.19                     | 0.42              |
| 11:A16:703:ALA:CA    | 24:D16:1398:ARG:CD   | 2.83                     | 0.42              |
| 17:F8:69:SER:HA      | 17:F8:70:PRO:HD3     | 1.81                     | 0.42              |
| 11:A32:642:GLY:O     | 11:A32:685:ARG:HD2   | 2.19                     | 0.42              |
| 18:B:437:PHE:CZ      | 18:B:473:LEU:HD13    | 2.54                     | 0.42              |
| 18:B:1098:MET:CE     | 18:B:1142:PHE:HB2    | 2.49                     | 0.42              |
| 18:B:1158:VAL:HG13   | 18:B:1338:GLN:O      | 2.19                     | 0.42              |
| 18:B:1372:THR:O      | 18:B:1376:ILE:HG13   | 2.19                     | 0.42              |
| 18:B8:132:LEU:HD11   | 18:B8:199:LEU:HD11   | 1.88                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:B8:326:PRO:HG2   | 18:B8:370:TYR:CD1   | 2.53                     | 0.42              |
| 18:B8:503:SER:N     | 18:B8:504:PRO:HD2   | 2.33                     | 0.42              |
| 18:B8:1783:VAL:HG21 | 18:B8:1810:VAL:HG21 | 2.01                     | 0.42              |
| 18:B8:1958:ALA:HB2  | 18:B8:1965:LEU:HD12 | 2.00                     | 0.42              |
| 19:4:421:GLN:HB3    | 19:4:440:ILE:HG23   | 2.01                     | 0.42              |
| 19:48:316:PHE:HB2   | 19:48:319:SER:HB3   | 2.01                     | 0.42              |
| 23:J24:733:ALA:HA   | 23:J24:734:PRO:HD3  | 1.47                     | 0.42              |
| 23:J16:679:GLU:C    | 23:J16:681:GLU:H    | 2.27                     | 0.42              |
| 24:D16:1112:ALA:HB2 | 24:D16:1160:LEU:CD1 | 2.45                     | 0.42              |
| 24:D32:1292:LYS:CE  | 24:D32:1337:ALA:HA  | 2.49                     | 0.42              |
| 10:C32:663:ILE:HG22 | 10:C32:667:ILE:HG21 | 2.00                     | 0.42              |
| 10:C32:750:TYR:OH   | 10:C32:813:LEU:HD23 | 2.19                     | 0.42              |
| 10:C32:1297:HIS:CE1 | 10:C32:1372:ALA:HB1 | 2.54                     | 0.42              |
| 2:M:624:ASP:OD1     | 2:M:624:ASP:N       | 2.50                     | 0.42              |
| 1:R16:1424:LYS:O    | 1:R16:1428:VAL:HG23 | 2.18                     | 0.42              |
| 7:Q:57:ASN:ND2      | 7:Q:62:HIS:CE1      | 2.87                     | 0.42              |
| 5:P16:16:PHE:HE1    | 6:O16:311:LEU:HD21  | 1.82                     | 0.42              |
| 5:P16:143:ASN:C     | 5:P16:145:ILE:H     | 2.27                     | 0.42              |
| 7:Q16:33:ARG:NH1    | 7:Q16:345:ASP:OD2   | 2.52                     | 0.42              |
| 8:L8:614:GLU:CD     | 8:L8:649:LYS:HZ3    | 2.27                     | 0.42              |
| 8:L16:1058:ILE:HG23 | 9:K16:1083:ILE:HD13 | 2.00                     | 0.42              |
| 9:K16:601:VAL:HG11  | 9:K16:673:SER:HB3   | 2.00                     | 0.42              |
| 10:C16:228:ARG:CZ   | 10:C16:277:SER:CB   | 2.94                     | 0.42              |
| 10:C16:1281:THR:O   | 10:C16:1284:ASP:HB2 | 2.20                     | 0.42              |
| 10:C16:1725:THR:C   | 10:C16:1727:SER:H   | 2.26                     | 0.42              |
| 10:C16:1757:GLN:OE1 | 11:A24:136:LEU:HD23 | 2.11                     | 0.42              |
| 11:A40:362:ARG:NE   | 11:A40:366:ARG:HH12 | 2.17                     | 0.42              |
| 11:A40:763:HIS:CE1  | 11:A40:815:VAL:HG21 | 2.55                     | 0.42              |
| 12:A:628:LEU:HG     | 12:A:637:LEU:HD12   | 2.00                     | 0.42              |
| 12:A:798:PHE:CE2    | 12:A:809:VAL:HG21   | 2.52                     | 0.42              |
| 10:C:228:ARG:CZ     | 10:C:277:SER:CB     | 2.94                     | 0.42              |
| 10:C:750:TYR:OH     | 10:C:813:LEU:HD23   | 2.19                     | 0.42              |
| 10:C:1059:ALA:O     | 10:C:1061:ASN:N     | 2.52                     | 0.42              |
| 10:C:1457:LEU:HD23  | 10:C:1521:ILE:HD13  | 2.00                     | 0.42              |
| 11:A16:362:ARG:NE   | 11:A16:366:ARG:HH12 | 2.17                     | 0.42              |
| 18:B:124:THR:C      | 18:B:126:GLU:N      | 2.77                     | 0.42              |
| 18:B:1415:LEU:CD1   | 18:B:1461:VAL:HG13  | 2.48                     | 0.42              |
| 18:B8:553:LEU:HD23  | 18:B8:558:VAL:CG2   | 2.49                     | 0.42              |
| 18:B8:671:MET:HE1   | 18:B8:736:ALA:HB3   | 1.94                     | 0.42              |
| 19:4:175:TYR:CZ     | 20:E:518:GLN:HG2    | 2.54                     | 0.42              |
| 20:E:6:VAL:CG1      | 20:E:7:PRO:HD2      | 2.50                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 20:E:331:GLY:HA2     | 20:E:357:PHE:CE2     | 2.54                     | 0.42              |
| 22:I24:206:PHE:O     | 22:I24:209:TRP:HB2   | 2.19                     | 0.42              |
| 22:I16:155:PHE:CZ    | 22:I16:159:ARG:HD2   | 2.51                     | 0.42              |
| 24:D8:1292:LYS:CE    | 24:D8:1337:ALA:HA    | 2.49                     | 0.42              |
| 24:D32:1325:ARG:C    | 24:D32:1326:ILE:HG13 | 2.44                     | 0.42              |
| 24:D40:7:ILE:HD12    | 24:D40:878:SER:CB    | 2.49                     | 0.42              |
| 24:D40:212:GLU:HB2   | 24:D40:230:LEU:HD11  | 2.01                     | 0.42              |
| 10:C32:698:PHE:CZ    | 10:C32:749:LEU:CD1   | 3.02                     | 0.42              |
| 10:C32:768:ARG:HD3   | 10:C32:778:GLU:HB2   | 2.01                     | 0.42              |
| 10:C32:1271:PHE:CD1  | 10:C32:1273:GLY:N    | 2.81                     | 0.42              |
| 10:C32:1424:GLN:HE22 | 10:C32:1478:VAL:HG13 | 1.81                     | 0.42              |
| 12:A48:375:ALA:N     | 12:A48:376:PRO:CD    | 2.81                     | 0.42              |
| 1:R:341:ARG:HH12     | 1:R:499:GLU:CD       | 2.28                     | 0.42              |
| 2:M:762:LEU:HD22     | 2:M:813:ASN:HD22     | 1.83                     | 0.42              |
| 2:M:816:ARG:HH22     | 2:M:849:LEU:HB3      | 1.83                     | 0.42              |
| 1:R8:341:ARG:HH12    | 1:R8:499:GLU:CD      | 2.28                     | 0.42              |
| 3:N8:135:ARG:NE      | 3:N8:141:ASP:OD1     | 2.49                     | 0.42              |
| 1:R16:422:ARG:HH22   | 1:R16:584:GLY:CA     | 2.32                     | 0.42              |
| 2:M16:843:ALA:O      | 4:T16:656:TRP:HH2    | 2.03                     | 0.42              |
| 5:P:143:ASN:C        | 5:P:145:ILE:H        | 2.27                     | 0.42              |
| 5:P:454:GLY:O        | 5:P:488:LYS:NZ       | 2.51                     | 0.42              |
| 5:P8:288:ARG:HB2     | 5:P8:289:PRO:HD2     | 2.02                     | 0.42              |
| 7:Q8:57:ASN:ND2      | 7:Q8:62:HIS:CE1      | 2.87                     | 0.42              |
| 7:Q16:57:ASN:ND2     | 7:Q16:62:HIS:CE1     | 2.87                     | 0.42              |
| 9:K:638:TRP:CH2      | 9:K:754:ARG:HD2      | 2.54                     | 0.42              |
| 9:K:736:LEU:HD21     | 9:K:770:VAL:HG13     | 2.02                     | 0.42              |
| 9:K8:577:GLN:CG      | 9:K8:625:ARG:NH1     | 2.81                     | 0.42              |
| 9:K8:745:ARG:HD2     | 9:K8:752:MET:HA      | 2.00                     | 0.42              |
| 9:K8:1048:GLN:OE1    | 9:K8:1128:ARG:CD     | 2.66                     | 0.42              |
| 10:C16:182:ASP:OD1   | 10:C16:182:ASP:N     | 2.52                     | 0.42              |
| 10:C16:275:ALA:CB    | 10:C16:326:LEU:CD1   | 2.96                     | 0.42              |
| 10:C16:323:HIS:HE1   | 10:C16:327:ILE:HD11  | 1.69                     | 0.42              |
| 10:C16:553:LEU:HD23  | 10:C16:595:THR:CG2   | 2.44                     | 0.42              |
| 10:C16:572:ILE:CG1   | 10:C16:606:MET:CE    | 2.90                     | 0.42              |
| 10:C16:855:VAL:N     | 10:C16:856:PRO:CD    | 2.82                     | 0.42              |
| 10:C16:1250:ALA:HB2  | 10:C16:1309:ARG:HH11 | 1.78                     | 0.42              |
| 10:C16:1263:LYS:HD3  | 10:C16:1263:LYS:HA   | 1.87                     | 0.42              |
| 10:C24:1257:ALA:C    | 10:C24:1323:LEU:HD11 | 2.43                     | 0.42              |
| 11:A40:780:LYS:HE2   | 24:D32:111:ASP:CG    | 2.43                     | 0.42              |
| 13:V:836:LEU:HD22    | 14:W:716:PHE:CD1     | 2.54                     | 0.42              |
| 10:C:736:ILE:CD1     | 10:C:794:LYS:HZ2     | 2.31                     | 0.42              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:1105:LEU:HD21  | 10:C:1183:LEU:HD21   | 2.01                     | 0.42              |
| 10:C:1129:VAL:CG1   | 10:C:1130:SER:N      | 2.81                     | 0.42              |
| 10:C:1271:PHE:CD1   | 10:C:1273:GLY:N      | 2.81                     | 0.42              |
| 10:C:1283:LEU:CD1   | 10:C:1357:LEU:HD13   | 2.49                     | 0.42              |
| 10:C8:102:ASN:HA    | 10:C8:107:LEU:HG     | 2.01                     | 0.42              |
| 10:C8:228:ARG:CZ    | 10:C8:277:SER:CB     | 2.94                     | 0.42              |
| 10:C8:667:ILE:CA    | 10:C8:670:GLU:H      | 2.32                     | 0.42              |
| 10:C8:1121:ILE:O    | 10:C8:1133:ILE:HD12  | 2.19                     | 0.42              |
| 10:C8:1163:LEU:C    | 10:C8:1166:SER:H     | 2.28                     | 0.42              |
| 10:C8:1265:ARG:HG2  | 10:C8:1268:ARG:HE    | 1.55                     | 0.42              |
| 10:C8:1457:LEU:HD23 | 10:C8:1521:ILE:HD13  | 2.00                     | 0.42              |
| 11:A16:609:ASN:OD1  | 11:A16:610:VAL:N     | 2.53                     | 0.42              |
| 11:A32:785:HIS:CG   | 11:A32:793:ALA:HB2   | 2.54                     | 0.42              |
| 18:B:86:LYS:CE      | 18:B:123:LEU:HD11    | 2.48                     | 0.42              |
| 18:B:429:GLY:H      | 18:B:475:GLU:CD      | 2.27                     | 0.42              |
| 18:B:472:SER:HA     | 18:B:584:ARG:HH12    | 1.84                     | 0.42              |
| 18:B:553:LEU:HD23   | 18:B:558:VAL:CG2     | 2.49                     | 0.42              |
| 18:B8:83:LEU:HD22   | 18:B8:105:VAL:HG12   | 2.00                     | 0.42              |
| 18:B8:243:GLY:CA    | 18:B8:248:SER:OG     | 2.67                     | 0.42              |
| 18:B8:377:SER:C     | 18:B8:379:LEU:N      | 2.78                     | 0.42              |
| 18:B8:429:GLY:H     | 18:B8:475:GLU:CD     | 2.27                     | 0.42              |
| 18:B8:1112:LYS:CE   | 21:H24:327:SER:CA    | 2.81                     | 0.42              |
| 18:B8:1205:ILE:HD12 | 18:B8:1271:PHE:CE2   | 2.53                     | 0.42              |
| 18:B8:1372:THR:O    | 18:B8:1376:ILE:HG13  | 2.20                     | 0.42              |
| 18:B8:1456:ASN:OD1  | 18:B8:1510:TYR:HD1   | 2.01                     | 0.42              |
| 18:B8:1660:SER:CA   | 18:B8:1724:MET:HE1   | 2.49                     | 0.42              |
| 19:4:17:ARG:NH2     | 19:4:386:ASP:OD2     | 2.51                     | 0.42              |
| 19:4:244:GLN:NE2    | 20:E:364:PHE:CE1     | 2.87                     | 0.42              |
| 19:4:294:SER:C      | 19:4:296:GLY:N       | 2.77                     | 0.42              |
| 20:E:347:PRO:C      | 20:E:349:THR:N       | 2.78                     | 0.42              |
| 19:48:125:ILE:CD1   | 19:48:139:LEU:HD11   | 2.49                     | 0.42              |
| 20:E8:6:VAL:CG1     | 20:E8:7:PRO:HD2      | 2.50                     | 0.42              |
| 21:H8:288:THR:CB    | 23:J8:650:GLN:NE2    | 2.75                     | 0.42              |
| 22:I8:199:PHE:HB3   | 23:J8:620:MET:CE     | 2.48                     | 0.42              |
| 21:H24:284:LEU:C    | 23:J24:650:GLN:NE2   | 2.77                     | 0.42              |
| 22:I16:321:LYS:HZ3  | 23:J16:711:GLU:HB2   | 1.83                     | 0.42              |
| 24:D24:1325:ARG:C   | 24:D24:1326:ILE:HG13 | 2.45                     | 0.42              |
| 24:D32:212:GLU:HB2  | 24:D32:230:LEU:HD11  | 2.01                     | 0.42              |
| 1:R:1002:ASP:CG     | 1:R:1024:ARG:HH21    | 2.27                     | 0.42              |
| 2:M:191:TRP:HH2     | 2:M:222:ILE:HD11     | 1.82                     | 0.42              |
| 2:M:742:PHE:HZ      | 2:M:801:GLU:OE2      | 2.03                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M8:731:ASN:CG      | 8:L16:504:GLN:HE22   | 2.27                     | 0.42              |
| 2:M16:632:VAL:HG22   | 3:N16:222:LEU:HB3    | 2.01                     | 0.42              |
| 3:N16:135:ARG:NE     | 3:N16:141:ASP:OD1    | 2.49                     | 0.42              |
| 5:P:43:TRP:CH2       | 5:P:76:LEU:HD12      | 2.55                     | 0.42              |
| 5:P:188:LEU:N        | 5:P:189:PRO:CD       | 2.83                     | 0.42              |
| 5:P:288:ARG:HB2      | 5:P:289:PRO:HD2      | 2.02                     | 0.42              |
| 7:Q:219:GLY:CA       | 7:Q:221:TRP:CD1      | 3.01                     | 0.42              |
| 5:P8:43:TRP:CH2      | 5:P8:76:LEU:HD12     | 2.55                     | 0.42              |
| 5:P8:206:SER:OG      | 5:P8:207:HIS:ND1     | 2.39                     | 0.42              |
| 5:P8:566:PHE:CZ      | 5:P8:597:GLY:O       | 2.71                     | 0.42              |
| 5:P16:262:ASP:OD1    | 5:P16:262:ASP:N      | 2.52                     | 0.42              |
| 7:Q16:149:VAL:HG23   | 7:Q16:187:TRP:NE1    | 2.35                     | 0.42              |
| 7:Q16:222:PHE:O      | 7:Q16:223:GLN:C      | 2.62                     | 0.42              |
| 9:K8:1066:ASP:O      | 9:K8:1068:GLN:N      | 2.51                     | 0.42              |
| 9:K16:788:LEU:HG     | 9:K16:856:ILE:HD11   | 2.01                     | 0.42              |
| 11:A24:736:PRO:CB    | 24:D16:871:ARG:NH1   | 2.79                     | 0.42              |
| 11:A24:763:HIS:CE1   | 11:A24:815:VAL:HG21  | 2.55                     | 0.42              |
| 11:A24:785:HIS:CG    | 11:A24:793:ALA:HB2   | 2.54                     | 0.42              |
| 10:C24:41:GLN:NE2    | 10:C24:165:ALA:HB1   | 2.34                     | 0.42              |
| 10:C24:445:MET:HE1   | 10:C24:462:PHE:HZ    | 1.84                     | 0.42              |
| 10:C24:515:ASP:O     | 10:C24:519:ILE:HG13  | 2.19                     | 0.42              |
| 10:C24:750:TYR:OH    | 10:C24:819:GLN:OE1   | 2.32                     | 0.42              |
| 10:C24:945:LEU:O     | 10:C24:993:HIS:HE1   | 2.03                     | 0.42              |
| 10:C24:1107:GLN:O    | 10:C24:1110:SER:CB   | 2.67                     | 0.42              |
| 10:C24:1163:LEU:HB3  | 10:C24:1166:SER:OG   | 2.19                     | 0.42              |
| 10:C24:1346:PHE:CD1  | 10:C24:1697:LEU:HD22 | 2.55                     | 0.42              |
| 10:C24:1385:LEU:HD11 | 10:C24:1419:PHE:HD1  | 1.84                     | 0.42              |
| 11:A40:849:TRP:HB2   | 11:A40:854:TYR:CE2   | 2.55                     | 0.42              |
| 12:A:609:ASN:OD1     | 12:A:610:VAL:N       | 2.53                     | 0.42              |
| 12:A:763:HIS:ND1     | 12:A:815:VAL:HG21    | 2.33                     | 0.42              |
| 13:V:902:MET:SD      | 14:W:781:LEU:HD12    | 2.59                     | 0.42              |
| 14:W:518:GLU:CG      | 14:W:605:ASN:HD21    | 2.29                     | 0.42              |
| 10:C:105:TRP:O       | 10:C:106:GLY:O       | 2.36                     | 0.42              |
| 10:C:698:PHE:CZ      | 10:C:749:LEU:CD1     | 3.02                     | 0.42              |
| 10:C:897:MET:HE1     | 10:C:961:GLY:HA2     | 2.02                     | 0.42              |
| 10:C:1121:ILE:O      | 10:C:1133:ILE:HD12   | 2.19                     | 0.42              |
| 10:C8:855:VAL:N      | 10:C8:856:PRO:HD2    | 2.35                     | 0.42              |
| 10:C8:1307:ILE:HG12  | 10:C8:1320:GLN:HB3   | 2.00                     | 0.42              |
| 10:C8:1317:ARG:HD3   | 10:C8:1387:LEU:HD21  | 2.01                     | 0.42              |
| 10:C8:1623:ILE:HG22  | 10:C8:1623:ILE:O     | 2.18                     | 0.42              |
| 18:B:154:LEU:HD22    | 18:B:224:GLU:CD      | 2.35                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:463:SER:OG      | 18:B:562:ARG:CZ      | 2.68                     | 0.42              |
| 18:B:1042:GLU:N      | 18:B:1043:PRO:CD     | 2.82                     | 0.42              |
| 18:B:1154:ILE:O      | 18:B:1158:VAL:HG23   | 2.20                     | 0.42              |
| 18:B8:124:THR:C      | 18:B8:126:GLU:N      | 2.77                     | 0.42              |
| 18:B8:349:PHE:CE1    | 18:B8:353:ILE:HD12   | 2.44                     | 0.42              |
| 18:B8:399:SER:OG     | 18:B8:444:VAL:O      | 2.24                     | 0.42              |
| 18:B8:789:LEU:CD1    | 18:B8:848:PHE:CE1    | 3.02                     | 0.42              |
| 22:I:321:LYS:NZ      | 23:J32:711:GLU:HB2   | 2.35                     | 0.42              |
| 22:I16:206:PHE:O     | 22:I16:209:TRP:HB2   | 2.19                     | 0.42              |
| 24:D:7:ILE:HD12      | 24:D:878:SER:CB      | 2.49                     | 0.42              |
| 24:D16:1170:VAL:HG22 | 24:D16:1232:VAL:HG22 | 2.01                     | 0.42              |
| 10:C32:424:ASP:HA    | 10:C32:425:PRO:HD3   | 1.81                     | 0.42              |
| 10:C32:750:TYR:OH    | 10:C32:819:GLN:OE1   | 2.32                     | 0.42              |
| 2:M:417:ARG:NH1      | 8:L:298:PHE:C        | 2.73                     | 0.42              |
| 2:M:420:CYS:HB3      | 8:L:391:TRP:HZ3      | 1.78                     | 0.42              |
| 2:M:443:ARG:HG2      | 2:M:448:ASP:OD2      | 2.20                     | 0.42              |
| 3:N:221:ASN:C        | 3:N:223:GLY:N        | 2.77                     | 0.42              |
| 2:M8:443:ARG:HG2     | 2:M8:448:ASP:OD2     | 2.20                     | 0.42              |
| 3:N8:278:ASP:OD1     | 3:N8:278:ASP:C       | 2.62                     | 0.42              |
| 1:R16:1002:ASP:CG    | 1:R16:1024:ARG:HH21  | 2.27                     | 0.42              |
| 1:R16:1132:TYR:OH    | 1:R16:1214:ILE:HD13  | 2.19                     | 0.42              |
| 2:M16:166:THR:N      | 2:M16:169:THR:HG1    | 2.12                     | 0.42              |
| 2:M16:185:ARG:HH11   | 2:M16:213:LEU:HD13   | 1.68                     | 0.42              |
| 2:M16:351:ALA:O      | 2:M16:353:ILE:N      | 2.52                     | 0.42              |
| 6:O:17:TRP:CE2       | 6:O:24:LEU:HD13      | 2.55                     | 0.42              |
| 5:P8:566:PHE:HE1     | 5:P8:600:PHE:HD1     | 1.68                     | 0.42              |
| 7:Q8:33:ARG:NH1      | 7:Q8:345:ASP:OD2     | 2.52                     | 0.42              |
| 5:P16:566:PHE:HE1    | 5:P16:600:PHE:HD1    | 1.68                     | 0.42              |
| 9:K8:1160:ARG:NH2    | 9:K8:1220:ASN:HD22   | 2.12                     | 0.42              |
| 10:C16:515:ASP:O     | 10:C16:519:ILE:HG13  | 2.19                     | 0.42              |
| 10:C16:547:VAL:HG21  | 10:C16:587:TYR:CD2   | 2.52                     | 0.42              |
| 10:C16:1502:ARG:O    | 10:C16:1504:ASP:N    | 2.53                     | 0.42              |
| 10:C16:1729:ASN:HB2  | 21:H:282:GLU:OE2     | 2.20                     | 0.42              |
| 10:C24:144:ASP:CB    | 10:C24:147:LEU:HD12  | 2.44                     | 0.42              |
| 10:C24:179:ASN:OD1   | 10:C24:213:ARG:NH1   | 2.52                     | 0.42              |
| 10:C24:855:VAL:N     | 10:C24:856:PRO:HD2   | 2.35                     | 0.42              |
| 11:A40:694:GLU:OE1   | 24:D24:1398:ARG:CA   | 2.56                     | 0.42              |
| 12:A:362:ARG:NE      | 12:A:366:ARG:HH12    | 2.17                     | 0.42              |
| 14:W:791:ASN:CB      | 15:J:706:ILE:HD13    | 2.50                     | 0.42              |
| 10:C:102:ASN:HA      | 10:C:107:LEU:HG      | 2.00                     | 0.42              |
| 10:C:573:GLU:OE1     | 10:C:617:TYR:OH      | 2.32                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:707:ILE:HD11    | 10:C:740:LEU:HD11    | 2.02                     | 0.42              |
| 10:C:855:VAL:N       | 10:C:856:PRO:CD      | 2.82                     | 0.42              |
| 10:C:1282:CYS:SG     | 10:C:1347:LEU:HD13   | 2.60                     | 0.42              |
| 10:C8:41:GLN:NE2     | 10:C8:165:ALA:HB1    | 2.34                     | 0.42              |
| 10:C8:515:ASP:O      | 10:C8:519:ILE:HG13   | 2.19                     | 0.42              |
| 10:C8:698:PHE:CZ     | 10:C8:749:LEU:CD1    | 3.02                     | 0.42              |
| 10:C8:1502:ARG:O     | 10:C8:1504:ASP:N     | 2.53                     | 0.42              |
| 11:A16:629:LEU:HD22  | 11:A16:675:LEU:HD12  | 2.01                     | 0.42              |
| 18:B:503:SER:N       | 18:B:504:PRO:HD2     | 2.33                     | 0.42              |
| 18:B:609:TYR:HD2     | 18:B:610:VAL:N       | 2.18                     | 0.42              |
| 18:B:1072:LEU:CD2    | 18:B:1076:GLU:OE2    | 2.56                     | 0.42              |
| 18:B8:1158:VAL:HG13  | 18:B8:1338:GLN:O     | 2.19                     | 0.42              |
| 18:B8:1424:LEU:HB3   | 18:B8:1486:ASP:HB3   | 2.02                     | 0.42              |
| 18:B8:1601:VAL:O     | 18:B8:1601:VAL:HG12  | 2.19                     | 0.42              |
| 20:E:201:LEU:C       | 20:E:203:TRP:N       | 2.77                     | 0.42              |
| 20:E8:346:GLN:HA     | 20:E8:347:PRO:HD3    | 1.88                     | 0.42              |
| 23:J8:733:ALA:HA     | 23:J8:734:PRO:HD3    | 1.47                     | 0.42              |
| 22:I24:321:LYS:NZ    | 23:J24:711:GLU:HB2   | 2.35                     | 0.42              |
| 22:I16:321:LYS:NZ    | 23:J16:711:GLU:HB2   | 2.35                     | 0.42              |
| 24:D8:212:GLU:HB2    | 24:D8:230:LEU:HD11   | 2.01                     | 0.42              |
| 24:D16:1325:ARG:C    | 24:D16:1326:ILE:HG13 | 2.44                     | 0.42              |
| 24:D24:212:GLU:HB2   | 24:D24:230:LEU:HD11  | 2.01                     | 0.42              |
| 10:C32:615:GLU:CA    | 10:C32:619:LEU:HD12  | 2.49                     | 0.42              |
| 10:C32:1062:GLU:HA   | 10:C32:1063:PRO:HD3  | 1.67                     | 0.42              |
| 10:C32:1283:LEU:CD1  | 10:C32:1357:LEU:HD13 | 2.49                     | 0.42              |
| 10:C32:1307:ILE:HG12 | 10:C32:1320:GLN:HB3  | 2.00                     | 0.42              |
| 10:C32:1317:ARG:HD3  | 10:C32:1387:LEU:HD21 | 2.01                     | 0.42              |
| 10:C32:1626:GLN:HE21 | 10:C32:1692:LYS:CE   | 2.31                     | 0.42              |
| 12:A48:362:ARG:NE    | 12:A48:366:ARG:HH12  | 2.17                     | 0.42              |
| 2:M:157:GLY:HA3      | 3:N:7:GLU:CD         | 2.44                     | 0.42              |
| 1:R8:1449:TRP:HH2    | 2:M8:161:ASP:N       | 2.17                     | 0.42              |
| 2:M8:401:ARG:HH22    | 8:L8:381:GLU:CB      | 2.28                     | 0.42              |
| 2:M8:742:PHE:HZ      | 2:M8:801:GLU:OE2     | 2.03                     | 0.42              |
| 2:M8:816:ARG:HH22    | 2:M8:849:LEU:HB3     | 1.83                     | 0.42              |
| 3:N8:97:HIS:HD2      | 3:N8:99:PHE:CZ       | 2.36                     | 0.42              |
| 2:M16:415:ASP:OD2    | 2:M16:456:ARG:NH2    | 2.43                     | 0.42              |
| 5:P:152:ILE:CG2      | 14:W:762:GLN:CD      | 2.89                     | 0.42              |
| 7:Q:172:LYS:HD3      | 7:Q:175:ASP:HB2      | 2.02                     | 0.42              |
| 5:P8:611:LEU:HG      | 5:P8:629:ARG:CG      | 2.46                     | 0.42              |
| 5:P8:634:MET:HE3     | 5:P8:674:LYS:HG3     | 2.01                     | 0.42              |
| 5:P16:214:LEU:HD21   | 5:P16:236:VAL:HG12   | 2.01                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:634:MET:HE3    | 5:P16:674:LYS:HG3    | 2.01                     | 0.42              |
| 8:L:1089:MET:CG      | 9:K:1000:SER:CB      | 2.95                     | 0.42              |
| 9:K8:1074:ARG:HH11   | 9:K8:1126:LEU:CD2    | 2.30                     | 0.42              |
| 10:C16:1107:GLN:O    | 10:C16:1110:SER:CB   | 2.67                     | 0.42              |
| 10:C16:1127:THR:O    | 10:C16:1128:SER:C    | 2.62                     | 0.42              |
| 10:C16:1724:VAL:CG2  | 10:C16:1736:ILE:HD12 | 2.47                     | 0.42              |
| 11:A24:362:ARG:NE    | 11:A24:366:ARG:HH12  | 2.17                     | 0.42              |
| 11:A24:642:GLY:O     | 11:A24:685:ARG:HD2   | 2.19                     | 0.42              |
| 10:C24:345:MET:HE1   | 10:C24:401:ILE:HD13  | 1.41                     | 0.42              |
| 10:C24:1157:LEU:HD22 | 10:C24:1176:VAL:HG11 | 2.01                     | 0.42              |
| 10:C24:1317:ARG:HD3  | 10:C24:1387:LEU:HD21 | 2.01                     | 0.42              |
| 11:A40:642:GLY:O     | 11:A40:685:ARG:HD2   | 2.19                     | 0.42              |
| 12:A:348:GLN:HB3     | 12:A:364:ILE:HD13    | 2.02                     | 0.42              |
| 14:W:130:VAL:CG2     | 14:W:151:ILE:HD11    | 2.42                     | 0.42              |
| 14:W:645:HIS:CE1     | 15:J:572:ASP:OD2     | 2.72                     | 0.42              |
| 14:W:701:LEU:HD13    | 15:J:624:ALA:CB      | 2.48                     | 0.42              |
| 10:C:41:GLN:NE2      | 10:C:165:ALA:HB1     | 2.34                     | 0.42              |
| 10:C:57:VAL:HG22     | 10:C:62:ILE:HD11     | 2.01                     | 0.42              |
| 10:C:398:SER:HA      | 10:C:458:VAL:HG11    | 2.01                     | 0.42              |
| 10:C:510:TRP:HB2     | 10:C:511:PRO:HD3     | 2.01                     | 0.42              |
| 10:C:515:ASP:O       | 10:C:519:ILE:HG13    | 2.19                     | 0.42              |
| 10:C:855:VAL:N       | 10:C:856:PRO:HD2     | 2.35                     | 0.42              |
| 10:C:1281:THR:O      | 10:C:1284:ASP:HB2    | 2.20                     | 0.42              |
| 10:C:1812:GLU:CG     | 10:C:1819:LEU:HD12   | 2.50                     | 0.42              |
| 10:C8:1297:HIS:CE1   | 10:C8:1372:ALA:HB1   | 2.54                     | 0.42              |
| 11:A16:823:VAL:O     | 11:A16:830:ILE:HD13  | 2.20                     | 0.42              |
| 11:A32:281:ARG:NH1   | 11:A32:381:TRP:CZ2   | 2.88                     | 0.42              |
| 11:A32:849:TRP:HB2   | 11:A32:854:TYR:CE2   | 2.55                     | 0.42              |
| 18:B:7:VAL:HG21      | 18:B:99:ILE:CD1      | 2.48                     | 0.42              |
| 18:B:377:SER:C       | 18:B:379:LEU:N       | 2.78                     | 0.42              |
| 18:B:671:MET:HE1     | 18:B:732:ASP:O       | 2.20                     | 0.42              |
| 18:B:690:TRP:HE3     | 18:B:739:VAL:CG2     | 1.94                     | 0.42              |
| 18:B:1248:LYS:HA     | 18:B:1252:ARG:O      | 2.19                     | 0.42              |
| 18:B8:154:LEU:HD22   | 18:B8:224:GLU:OE1    | 2.19                     | 0.42              |
| 18:B8:463:SER:OG     | 18:B8:562:ARG:CZ     | 2.68                     | 0.42              |
| 18:B8:678:PRO:C      | 18:B8:680:SER:H      | 2.27                     | 0.42              |
| 18:B8:1270:SER:HB2   | 18:B8:1273:GLU:HB2   | 2.01                     | 0.42              |
| 20:E8:166:PRO:HA     | 20:E8:167:PRO:HD3    | 1.94                     | 0.42              |
| 20:E8:331:GLY:HA2    | 20:E8:357:PHE:CE2    | 2.55                     | 0.42              |
| 22:I:206:PHE:O       | 22:I:209:TRP:HB2     | 2.20                     | 0.42              |
| 21:H16:267:LYS:HZ2   | 23:J16:631:GLU:HB3   | 1.85                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I16:97:THR:HG22   | 22:I16:107:THR:CG2   | 2.48                     | 0.42              |
| 22:I16:368:VAL:HG22  | 23:J16:591:LYS:NZ    | 2.35                     | 0.42              |
| 24:D40:1170:VAL:HG22 | 24:D40:1232:VAL:HG22 | 2.01                     | 0.42              |
| 10:C32:1107:GLN:O    | 10:C32:1110:SER:CB   | 2.67                     | 0.42              |
| 12:A48:628:LEU:HG    | 12:A48:637:LEU:HD12  | 2.00                     | 0.42              |
| 1:R:1166:ASN:ND2     | 5:P:672:LEU:CD2      | 2.63                     | 0.42              |
| 1:R:1180:PRO:HB3     | 1:R:1211:LYS:HB3     | 2.02                     | 0.42              |
| 1:R:1335:ILE:HD11    | 10:C:1170:VAL:CG1    | 2.50                     | 0.42              |
| 2:M:250:LEU:CD1      | 2:M:286:SER:HB3      | 2.40                     | 0.42              |
| 2:M:414:GLY:HA2      | 8:L:401:LYS:NZ       | 2.35                     | 0.42              |
| 3:N:116:ILE:HG21     | 3:N:177:TYR:CE1      | 2.51                     | 0.42              |
| 2:M8:351:ALA:O       | 2:M8:353:ILE:N       | 2.51                     | 0.42              |
| 2:M16:191:TRP:HH2    | 2:M16:222:ILE:HD11   | 1.82                     | 0.42              |
| 2:M16:742:PHE:HZ     | 2:M16:801:GLU:OE2    | 2.03                     | 0.42              |
| 5:P:233:TYR:CZ       | 5:P:237:MET:CE       | 3.03                     | 0.42              |
| 7:Q:33:ARG:NH1       | 7:Q:345:ASP:OD2      | 2.52                     | 0.42              |
| 7:Q:254:ALA:CB       | 7:Q:302:ILE:CD1      | 2.97                     | 0.42              |
| 5:P8:143:ASN:C       | 5:P8:145:ILE:H       | 2.27                     | 0.42              |
| 5:P8:465:TYR:CE1     | 5:P8:482:TYR:CZ      | 3.07                     | 0.42              |
| 5:P16:106:ARG:NH1    | 5:P16:458:GLU:OE1    | 2.52                     | 0.42              |
| 7:Q16:254:ALA:CB     | 7:Q16:302:ILE:CD1    | 2.97                     | 0.42              |
| 9:K:745:ARG:CG       | 9:K:752:MET:HA       | 2.48                     | 0.42              |
| 9:K:1110:GLN:HA      | 9:K:1132:LEU:HD21    | 2.02                     | 0.42              |
| 9:K8:691:LEU:CD1     | 9:K8:820:TYR:HA      | 2.49                     | 0.42              |
| 9:K8:971:LEU:O       | 9:K8:975:MET:HG3     | 2.20                     | 0.42              |
| 9:K8:1153:ALA:CA     | 9:K8:1220:ASN:ND2    | 2.83                     | 0.42              |
| 10:C16:31:HIS:CE1    | 10:C16:35:ASN:HD21   | 2.38                     | 0.42              |
| 10:C16:698:PHE:CZ    | 10:C16:749:LEU:CD1   | 3.02                     | 0.42              |
| 10:C16:879:LEU:CD2   | 10:C16:944:MET:HG3   | 2.49                     | 0.42              |
| 10:C16:1385:LEU:HD11 | 10:C16:1419:PHE:HD1  | 1.84                     | 0.42              |
| 10:C16:1547:LYS:HD3  | 24:D8:1406:SER:CB    | 2.50                     | 0.42              |
| 10:C16:1626:GLN:NE2  | 10:C16:1692:LYS:HZ3  | 2.06                     | 0.42              |
| 11:A24:281:ARG:NH1   | 11:A24:381:TRP:CZ2   | 2.88                     | 0.42              |
| 11:A24:348:GLN:HB3   | 11:A24:364:ILE:HD13  | 2.02                     | 0.42              |
| 11:A24:629:LEU:C     | 11:A24:678:LYS:HZ2   | 2.12                     | 0.42              |
| 10:C24:265:PHE:O     | 10:C24:269:ILE:HG13  | 2.20                     | 0.42              |
| 10:C24:971:ASP:HA    | 10:C24:972:PRO:HD3   | 1.89                     | 0.42              |
| 10:C24:1691:GLU:OE2  | 23:J24:735:LYS:HG2   | 2.20                     | 0.42              |
| 11:A40:281:ARG:NH1   | 11:A40:381:TRP:CZ2   | 2.88                     | 0.42              |
| 11:A40:348:GLN:HB3   | 11:A40:364:ILE:HD13  | 2.02                     | 0.42              |
| 11:A40:609:ASN:OD1   | 11:A40:610:VAL:N     | 2.53                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:A:763:HIS:CE1    | 12:A:815:VAL:HG21   | 2.55                     | 0.42              |
| 13:V:811:MET:HE2    | 13:V:811:MET:HB3    | 1.76                     | 0.42              |
| 10:C:182:ASP:OD1    | 10:C:182:ASP:N      | 2.52                     | 0.42              |
| 10:C:768:ARG:HD3    | 10:C:778:GLU:HB2    | 2.01                     | 0.42              |
| 10:C:1280:VAL:HA    | 10:C:1731:HIS:HE1   | 1.85                     | 0.42              |
| 10:C8:898:GLN:CD    | 10:C8:1138:GLU:OE2  | 2.47                     | 0.42              |
| 10:C8:1162:PRO:C    | 10:C8:1164:VAL:H    | 2.28                     | 0.42              |
| 10:C8:1271:PHE:CE2  | 10:C8:1284:ASP:CA   | 2.99                     | 0.42              |
| 10:C8:1281:THR:O    | 10:C8:1284:ASP:HB2  | 2.20                     | 0.42              |
| 10:C8:1344:VAL:HG12 | 10:C8:1348:LEU:HD12 | 2.02                     | 0.42              |
| 11:A16:281:ARG:NH1  | 11:A16:381:TRP:CZ2  | 2.88                     | 0.42              |
| 11:A16:763:HIS:CE1  | 11:A16:815:VAL:HG21 | 2.55                     | 0.42              |
| 11:A16:849:TRP:HB2  | 11:A16:854:TYR:CE2  | 2.55                     | 0.42              |
| 18:B:34:GLN:N       | 18:B:35:PRO:HD2     | 2.34                     | 0.42              |
| 18:B:809:THR:HG23   | 18:B:871:ILE:HD12   | 2.02                     | 0.42              |
| 18:B8:671:MET:HE1   | 18:B8:732:ASP:O     | 2.20                     | 0.42              |
| 18:B8:729:LEU:CB    | 18:B8:1196:MET:HE3  | 2.44                     | 0.42              |
| 18:B8:1042:GLU:N    | 18:B8:1043:PRO:CD   | 2.82                     | 0.42              |
| 19:4:269:PHE:HB3    | 19:4:281:TRP:HB2    | 2.00                     | 0.42              |
| 20:E:429:PRO:CG     | 24:D:69:VAL:CG2     | 2.92                     | 0.42              |
| 19:48:38:LEU:HD11   | 19:48:438:PRO:HB3   | 2.02                     | 0.42              |
| 19:48:403:GLY:HA3   | 19:48:429:TRP:CE2   | 2.54                     | 0.42              |
| 20:E8:343:THR:HA    | 20:E8:344:PRO:HD3   | 1.60                     | 0.42              |
| 21:H:267:LYS:HZ2    | 23:J32:631:GLU:HB3  | 1.84                     | 0.42              |
| 22:I8:206:PHE:O     | 22:I8:209:TRP:HB2   | 2.19                     | 0.42              |
| 22:I16:203:GLN:CD   | 22:I16:209:TRP:HZ2  | 2.19                     | 0.42              |
| 10:C32:47:PRO:HG2   | 10:C32:93:ASP:OD2   | 2.19                     | 0.42              |
| 10:C32:987:TYR:O    | 10:C32:988:GLN:C    | 2.62                     | 0.42              |
| 10:C32:1280:VAL:HA  | 10:C32:1731:HIS:HE1 | 1.85                     | 0.42              |
| 10:C32:1281:THR:O   | 10:C32:1284:ASP:HB2 | 2.20                     | 0.42              |
| 12:A48:609:ASN:OD1  | 12:A48:610:VAL:N    | 2.52                     | 0.42              |
| 12:A48:696:ILE:HD11 | 12:A48:728:ILE:HD12 | 1.92                     | 0.42              |
| 12:A48:823:VAL:O    | 12:A48:830:ILE:HD13 | 2.20                     | 0.42              |
| 2:M8:627:TYR:HD2    | 3:N8:167:LEU:CA     | 2.22                     | 0.42              |
| 1:R16:1444:VAL:HG11 | 1:R16:1475:LEU:HD11 | 2.01                     | 0.42              |
| 2:M16:416:VAL:HG13  | 8:L16:394:ALA:O     | 2.19                     | 0.42              |
| 5:P:16:PHE:HE1      | 6:O:311:LEU:HD21    | 1.82                     | 0.42              |
| 5:P:645:LEU:N       | 5:P:646:PRO:CD      | 2.82                     | 0.42              |
| 5:P8:188:LEU:N      | 5:P8:189:PRO:CD     | 2.83                     | 0.42              |
| 7:Q8:236:HIS:NE2    | 7:Q8:303:LEU:CD1    | 2.83                     | 0.42              |
| 5:P16:105:ARG:CZ    | 5:P16:133:TYR:HD1   | 2.19                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:645:LEU:N      | 5:P16:646:PRO:CD     | 2.82                     | 0.42              |
| 9:K:691:LEU:CD1      | 9:K:820:TYR:HA       | 2.49                     | 0.42              |
| 9:K16:1056:VAL:HG12  | 9:K16:1057:GLU:HG3   | 2.01                     | 0.42              |
| 10:C16:1163:LEU:HB3  | 10:C16:1166:SER:OG   | 2.19                     | 0.42              |
| 10:C16:1282:CYS:SG   | 10:C16:1347:LEU:HD13 | 2.60                     | 0.42              |
| 10:C16:1477:GLN:CG   | 24:D8:1407:PHE:CD1   | 3.03                     | 0.42              |
| 11:A24:401:GLU:HG3   | 11:A24:405:ARG:HE    | 1.85                     | 0.42              |
| 11:A24:849:TRP:HB2   | 11:A24:854:TYR:CE2   | 2.55                     | 0.42              |
| 10:C24:323:HIS:HE1   | 10:C24:327:ILE:HD11  | 1.68                     | 0.42              |
| 10:C24:768:ARG:HD3   | 10:C24:778:GLU:HB2   | 2.01                     | 0.42              |
| 10:C24:1219:ILE:CD1  | 10:C24:1229:LEU:HD21 | 2.50                     | 0.42              |
| 10:C24:1263:LYS:HD3  | 10:C24:1263:LYS:HA   | 1.88                     | 0.42              |
| 10:C24:1282:CYS:SG   | 10:C24:1347:LEU:HD13 | 2.60                     | 0.42              |
| 10:C24:1449:GLU:OE1  | 24:D24:1151:SER:HA   | 2.20                     | 0.42              |
| 10:C24:1502:ARG:O    | 10:C24:1504:ASP:N    | 2.53                     | 0.42              |
| 10:C24:1682:VAL:HG22 | 10:C24:1758:LEU:HD23 | 1.89                     | 0.42              |
| 12:A:281:ARG:NH1     | 12:A:381:TRP:CZ2     | 2.88                     | 0.42              |
| 13:V:878:ALA:C       | 13:V:880:ARG:N       | 2.78                     | 0.42              |
| 10:C:47:PRO:HG2      | 10:C:93:ASP:OD2      | 2.19                     | 0.42              |
| 10:C:1219:ILE:CD1    | 10:C:1229:LEU:HD21   | 2.50                     | 0.42              |
| 10:C:1346:PHE:CD1    | 10:C:1697:LEU:HD22   | 2.55                     | 0.42              |
| 10:C:1385:LEU:HD11   | 10:C:1419:PHE:HD1    | 1.84                     | 0.42              |
| 10:C8:168:ARG:HH22   | 10:C8:227:ASP:C      | 2.23                     | 0.42              |
| 10:C8:265:PHE:O      | 10:C8:269:ILE:HG13   | 2.20                     | 0.42              |
| 10:C8:390:HIS:CE1    | 10:C8:459:LEU:HD12   | 2.54                     | 0.42              |
| 10:C8:768:ARG:HD3    | 10:C8:778:GLU:HB2    | 2.01                     | 0.42              |
| 10:C8:837:ARG:CZ     | 10:C8:890:ASP:CB     | 2.92                     | 0.42              |
| 10:C8:897:MET:HE1    | 10:C8:961:GLY:HA2    | 2.02                     | 0.42              |
| 10:C8:1346:PHE:CD1   | 10:C8:1697:LEU:HD22  | 2.55                     | 0.42              |
| 10:C8:1560:GLN:OE1   | 10:C8:1601:TYR:HD1   | 1.96                     | 0.42              |
| 11:A32:629:LEU:HD22  | 11:A32:675:LEU:HD12  | 2.01                     | 0.42              |
| 18:B:678:PRO:C       | 18:B:680:SER:H       | 2.27                     | 0.42              |
| 18:B:842:ASN:C       | 18:B:899:LYS:HZ2     | 2.22                     | 0.42              |
| 18:B:1270:SER:HB2    | 18:B:1273:GLU:HB2    | 2.01                     | 0.42              |
| 18:B8:90:ILE:HD11    | 18:B8:131:ILE:HD13   | 2.02                     | 0.42              |
| 18:B8:409:LEU:O      | 18:B8:462:ARG:NH2    | 2.53                     | 0.42              |
| 20:E:6:VAL:O         | 20:E:9:THR:OG1       | 2.30                     | 0.42              |
| 20:E8:408:LEU:HD12   | 20:E8:507:LEU:HD23   | 2.01                     | 0.42              |
| 20:E8:418:THR:C      | 20:E8:420:LEU:N      | 2.73                     | 0.42              |
| 22:I:307:VAL:O       | 22:I:311:VAL:HG23    | 2.19                     | 0.42              |
| 21:H24:139:ASP:HA    | 21:H24:140:PRO:HD3   | 1.96                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 22:I24:97:THR:HG22   | 22:I24:107:THR:CG2   | 2.48                     | 0.42              |
| 21:H16:255:LEU:CD1   | 23:J16:655:GLU:CD    | 2.85                     | 0.42              |
| 21:H16:261:ILE:HD12  | 22:I16:195:ALA:HB1   | 2.02                     | 0.42              |
| 24:D8:94:ALA:HB1     | 24:D8:543:MET:HE1    | 2.00                     | 0.42              |
| 24:D8:853:MET:CB     | 24:D8:885:TYR:CD2    | 3.03                     | 0.42              |
| 24:D16:212:GLU:HB2   | 24:D16:230:LEU:HD11  | 2.01                     | 0.42              |
| 24:D24:472:ILE:HD11  | 24:D24:539:THR:CG2   | 2.48                     | 0.42              |
| 24:D24:1284:ILE:HD11 | 24:D24:1319:ALA:HA   | 2.01                     | 0.42              |
| 10:C32:265:PHE:O     | 10:C32:269:ILE:HG13  | 2.20                     | 0.42              |
| 10:C32:667:ILE:CA    | 10:C32:670:GLU:H     | 2.32                     | 0.42              |
| 10:C32:945:LEU:O     | 10:C32:993:HIS:HE1   | 2.03                     | 0.42              |
| 10:C32:1121:ILE:O    | 10:C32:1133:ILE:HD12 | 2.19                     | 0.42              |
| 12:A48:232:ASP:O     | 12:A48:236:THR:HG23  | 2.20                     | 0.42              |
| 1:R:983:ARG:HD3      | 24:D:1364:PRO:O      | 2.19                     | 0.42              |
| 1:R:1431:ARG:O       | 2:M:177:VAL:HG11     | 2.19                     | 0.42              |
| 2:M:625:HIS:NE2      | 3:N:225:PRO:HB3      | 2.34                     | 0.42              |
| 2:M:783:TRP:HB3      | 2:M:787:LEU:HG       | 2.02                     | 0.42              |
| 2:M8:157:GLY:HA3     | 3:N8:7:GLU:CD        | 2.44                     | 0.42              |
| 2:M8:294:GLN:O       | 2:M8:300:LEU:HD11    | 2.20                     | 0.42              |
| 3:N8:301:GLU:HA      | 3:N8:302:PRO:HD3     | 1.91                     | 0.42              |
| 1:R16:1431:ARG:O     | 2:M16:177:VAL:HG11   | 2.20                     | 0.42              |
| 3:N16:200:MET:CE     | 3:N16:203:PHE:CD2    | 2.96                     | 0.42              |
| 6:O:120:LYS:HG3      | 10:C:1163:LEU:CD1    | 2.49                     | 0.42              |
| 7:Q:149:VAL:HG23     | 7:Q:187:TRP:NE1      | 2.35                     | 0.42              |
| 5:P16:188:LEU:N      | 5:P16:189:PRO:CD     | 2.83                     | 0.42              |
| 9:K:585:GLU:CA       | 9:K:622:VAL:HG13     | 2.49                     | 0.42              |
| 9:K:786:GLN:HE22     | 9:K:794:ARG:HH11     | 1.66                     | 0.42              |
| 9:K:1153:ALA:CA      | 9:K:1220:ASN:ND2     | 2.83                     | 0.42              |
| 10:C16:57:VAL:HG22   | 10:C16:62:ILE:HD11   | 2.01                     | 0.42              |
| 10:C16:987:TYR:O     | 10:C16:988:GLN:C     | 2.62                     | 0.42              |
| 10:C16:1219:ILE:CD1  | 10:C16:1229:LEU:HD21 | 2.50                     | 0.42              |
| 11:A24:157:LEU:HD22  | 11:A24:523:LYS:HZ3   | 1.84                     | 0.42              |
| 11:A24:609:ASN:OD1   | 11:A24:610:VAL:N     | 2.53                     | 0.42              |
| 11:A24:694:GLU:OE2   | 24:D8:1397:THR:CA    | 2.67                     | 0.42              |
| 11:A24:794:THR:C     | 11:A24:796:ASP:N     | 2.77                     | 0.42              |
| 10:C24:57:VAL:HG22   | 10:C24:62:ILE:HD11   | 2.01                     | 0.42              |
| 10:C24:750:TYR:OH    | 10:C24:813:LEU:HD23  | 2.19                     | 0.42              |
| 10:C24:919:ASP:H     | 10:C24:927:THR:HG23  | 1.84                     | 0.42              |
| 10:C24:1280:VAL:HA   | 10:C24:1731:HIS:HE1  | 1.85                     | 0.42              |
| 10:C24:1507:LEU:C    | 10:C24:1509:SER:N    | 2.67                     | 0.42              |
| 10:C24:1547:LYS:CE   | 24:D24:1405:GLY:CA   | 2.98                     | 0.42              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C24:1708:ARG:CA  | 10:C24:1730:ILE:HD11 | 2.48                     | 0.42              |
| 10:C24:1725:THR:C   | 10:C24:1727:SER:N    | 2.77                     | 0.42              |
| 11:A40:11:THR:HG21  | 22:I16:162:GLN:CD    | 2.41                     | 0.42              |
| 11:A40:737:GLU:CG   | 24:D32:802:PHE:CE2   | 3.03                     | 0.42              |
| 14:W:425:THR:C      | 14:W:427:ASN:H       | 2.28                     | 0.42              |
| 14:W:717:LYS:HZ2    | 15:J:643:THR:HG23    | 1.85                     | 0.42              |
| 10:C:615:GLU:C      | 10:C:619:LEU:HD12    | 2.45                     | 0.42              |
| 10:C:1309:ARG:NE    | 10:C:1311:GLU:O      | 2.53                     | 0.42              |
| 10:C8:1059:ALA:O    | 10:C8:1061:ASN:N     | 2.52                     | 0.42              |
| 10:C8:1107:GLN:O    | 10:C8:1110:SER:CB    | 2.67                     | 0.42              |
| 10:C8:1282:CYS:SG   | 10:C8:1347:LEU:HD13  | 2.60                     | 0.42              |
| 10:C8:1586:VAL:HG21 | 10:C8:1635:LEU:HD11  | 2.02                     | 0.42              |
| 11:A32:676:TYR:CD2  | 24:D32:1396:PRO:HD2  | 2.45                     | 0.42              |
| 11:A32:698:LYS:CD   | 11:A32:804:TYR:CE1   | 3.02                     | 0.42              |
| 18:B:90:ILE:HD11    | 18:B:131:ILE:HD13    | 2.02                     | 0.42              |
| 18:B:477:SER:HA     | 18:B:588:PHE:O       | 2.19                     | 0.42              |
| 18:B:968:PHE:HB3    | 18:B:1040:MET:HE2    | 2.00                     | 0.42              |
| 18:B8:609:TYR:HD2   | 18:B8:610:VAL:N      | 2.18                     | 0.42              |
| 18:B8:628:VAL:HA    | 18:B8:631:LEU:CD1    | 2.50                     | 0.42              |
| 18:B8:690:TRP:CZ3   | 18:B8:787:VAL:HG13   | 2.54                     | 0.42              |
| 18:B8:980:LYS:O     | 18:B8:981:GLN:C      | 2.63                     | 0.42              |
| 18:B8:1209:LEU:HD23 | 18:B8:1238:PHE:HE1   | 1.84                     | 0.42              |
| 19:48:65:LYS:C      | 19:48:66:ALA:O       | 2.61                     | 0.42              |
| 20:E8:339:LYS:C     | 20:E8:340:GLY:O      | 2.63                     | 0.42              |
| 20:E8:434:TRP:NE1   | 24:D40:72:GLU:HB2    | 2.07                     | 0.42              |
| 24:D:1325:ARG:C     | 24:D:1326:ILE:HG13   | 2.44                     | 0.42              |
| 10:C32:515:ASP:O    | 10:C32:519:ILE:HG13  | 2.19                     | 0.42              |
| 10:C32:747:LYS:HB3  | 10:C32:748:ALA:H     | 1.68                     | 0.42              |
| 10:C32:897:MET:HE1  | 10:C32:961:GLY:HA2   | 2.02                     | 0.42              |
| 10:C32:1163:LEU:HB3 | 10:C32:1166:SER:OG   | 2.19                     | 0.42              |
| 10:C32:1309:ARG:NE  | 10:C32:1311:GLU:O    | 2.53                     | 0.42              |
| 10:C32:1619:PRO:HB2 | 10:C32:1621:LYS:HG3  | 2.00                     | 0.42              |
| 10:C32:1662:ASP:HB3 | 10:C32:1663:SER:H    | 1.61                     | 0.42              |
| 1:R:768:LEU:HD21    | 24:D:1362:VAL:HG13   | 2.01                     | 0.41              |
| 2:M:174:ARG:O       | 3:N:212:TRP:HH2      | 2.03                     | 0.41              |
| 2:M:198:PHE:CE1     | 2:M:219:LYS:HG3      | 2.55                     | 0.41              |
| 1:R8:1242:SER:HG    | 1:R8:1244:LEU:HD12   | 1.84                     | 0.41              |
| 2:M8:540:TYR:HB3    | 2:M8:558:MET:SD      | 2.60                     | 0.41              |
| 2:M16:691:TRP:CE2   | 2:M16:725:ARG:HG3    | 2.55                     | 0.41              |
| 7:Q:236:HIS:NE2     | 7:Q:303:LEU:CD1      | 2.83                     | 0.41              |
| 5:P8:233:TYR:CZ     | 5:P8:237:MET:CE      | 3.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:P8:402:LEU:CD1    | 5:P8:433:LEU:HD13   | 2.50                     | 0.41              |
| 6:O8:286:MET:HB3    | 6:O8:295:LEU:HD11   | 2.01                     | 0.41              |
| 6:O16:17:TRP:CE2    | 6:O16:24:LEU:HD13   | 2.55                     | 0.41              |
| 9:K8:743:ARG:NH1    | 9:K8:772:TYR:CD1    | 2.75                     | 0.41              |
| 9:K8:840:TRP:CZ3    | 9:K8:907:ILE:HG13   | 2.54                     | 0.41              |
| 9:K16:774:LEU:HD22  | 9:K16:842:ILE:HD11  | 2.02                     | 0.41              |
| 10:C16:1333:HIS:ND1 | 10:C16:1337:LEU:HB2 | 2.35                     | 0.41              |
| 10:C16:1725:THR:C   | 10:C16:1727:SER:N   | 2.77                     | 0.41              |
| 10:C24:31:HIS:CE1   | 10:C24:35:ASN:HD21  | 2.38                     | 0.41              |
| 10:C24:300:VAL:HG12 | 10:C24:317:ARG:HG2  | 1.99                     | 0.41              |
| 10:C24:368:VAL:O    | 10:C24:371:THR:OG1  | 2.36                     | 0.41              |
| 12:A:823:VAL:O      | 12:A:830:ILE:HD13   | 2.20                     | 0.41              |
| 13:V:772:GLY:HA3    | 14:W:660:LEU:HD21   | 2.01                     | 0.41              |
| 14:W:698:LEU:HD11   | 15:J:621:GLU:HG3    | 2.01                     | 0.41              |
| 10:C:1109:VAL:C     | 10:C:1111:SER:H     | 2.27                     | 0.41              |
| 10:C:1163:LEU:C     | 10:C:1166:SER:H     | 2.28                     | 0.41              |
| 10:C:1599:ASP:OD2   | 10:C:1604:VAL:CB    | 2.66                     | 0.41              |
| 10:C8:919:ASP:H     | 10:C8:927:THR:HG23  | 1.84                     | 0.41              |
| 10:C8:1530:PHE:CE1  | 16:A8:132:MET:CE    | 2.92                     | 0.41              |
| 11:A16:98:ALA:O     | 18:B:1103:LYS:CE    | 2.68                     | 0.41              |
| 11:A16:232:ASP:O    | 11:A16:236:THR:HG23 | 2.20                     | 0.41              |
| 11:A16:676:TYR:CE2  | 24:D16:1395:SER:C   | 2.93                     | 0.41              |
| 11:A32:10:TRP:HH2   | 21:H24:338:MET:HE3  | 1.85                     | 0.41              |
| 11:A32:763:HIS:CE1  | 11:A32:815:VAL:HG21 | 2.55                     | 0.41              |
| 18:B:1424:LEU:HB3   | 18:B:1486:ASP:HB3   | 2.02                     | 0.41              |
| 18:B:1456:ASN:OD1   | 18:B:1510:TYR:CD1   | 2.73                     | 0.41              |
| 18:B8:132:LEU:HD13  | 18:B8:199:LEU:CD1   | 2.45                     | 0.41              |
| 18:B8:1248:LYS:HA   | 18:B8:1252:ARG:O    | 2.19                     | 0.41              |
| 18:B8:1731:PHE:CZ   | 18:B8:1749:LEU:HD13 | 2.55                     | 0.41              |
| 20:E:84:GLY:HA3     | 20:E:94:PHE:CZ      | 2.55                     | 0.41              |
| 20:E:148:VAL:O      | 20:E:152:THR:HG23   | 2.20                     | 0.41              |
| 20:E:204:SER:O      | 20:E:205:GLY:C      | 2.58                     | 0.41              |
| 20:E:341:TYR:C      | 20:E:342:GLN:O      | 2.62                     | 0.41              |
| 19:48:340:PRO:CD    | 24:D8:140:ALA:CB    | 2.92                     | 0.41              |
| 20:E8:204:SER:O     | 20:E8:205:GLY:C     | 2.58                     | 0.41              |
| 21:H:141:THR:O      | 21:H:143:PRO:HD3    | 2.20                     | 0.41              |
| 23:J32:679:GLU:C    | 23:J32:681:GLU:H    | 2.27                     | 0.41              |
| 21:H24:141:THR:O    | 21:H24:143:PRO:HD3  | 2.20                     | 0.41              |
| 23:J24:679:GLU:C    | 23:J24:681:GLU:H    | 2.27                     | 0.41              |
| 22:I16:307:VAL:O    | 22:I16:311:VAL:HG23 | 2.19                     | 0.41              |
| 24:D:1102:VAL:HA    | 24:D:1153:GLN:HG2   | 2.02                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:761:VAL:HG21  | 10:C32:826:TYR:CA    | 2.42                     | 0.41              |
| 10:C32:798:VAL:HG11  | 10:C32:802:TRP:CE2   | 2.50                     | 0.41              |
| 1:R:1229:GLU:HG3     | 1:R:1239:TRP:O       | 2.20                     | 0.41              |
| 2:M:294:GLN:O        | 2:M:300:LEU:HD11     | 2.20                     | 0.41              |
| 2:M:691:TRP:CE2      | 2:M:725:ARG:HG3      | 2.55                     | 0.41              |
| 1:R8:1002:ASP:CG     | 1:R8:1024:ARG:HH21   | 2.27                     | 0.41              |
| 1:R8:1265:PHE:CE2    | 5:P8:684:ARG:CD      | 2.85                     | 0.41              |
| 2:M8:198:PHE:CE1     | 2:M8:219:LYS:HG3     | 2.55                     | 0.41              |
| 1:R16:1180:PRO:HB3   | 1:R16:1211:LYS:HB3   | 2.02                     | 0.41              |
| 2:M16:294:GLN:O      | 2:M16:300:LEU:HD11   | 2.20                     | 0.41              |
| 5:P:55:ARG:HH22      | 5:P:62:ASP:HB2       | 1.85                     | 0.41              |
| 6:O8:82:LEU:HD23     | 6:O8:103:MET:HE1     | 1.87                     | 0.41              |
| 7:Q8:149:VAL:HG23    | 7:Q8:187:TRP:NE1     | 2.35                     | 0.41              |
| 5:P16:43:TRP:CH2     | 5:P16:76:LEU:HD12    | 2.55                     | 0.41              |
| 6:O16:294:THR:OG1    | 6:O16:308:GLN:NE2    | 2.31                     | 0.41              |
| 7:Q16:32:ASN:HB3     | 7:Q16:34:PHE:CZ      | 2.55                     | 0.41              |
| 9:K:697:LEU:HA       | 9:K:764:VAL:HG11     | 2.02                     | 0.41              |
| 9:K:1171:TRP:CZ3     | 9:K:1206:LEU:HD23    | 2.56                     | 0.41              |
| 9:K8:751:LEU:CD2     | 9:K8:754:ARG:CD      | 2.97                     | 0.41              |
| 9:K8:1150:GLU:OE1    | 9:K8:1212:ARG:CZ     | 2.68                     | 0.41              |
| 9:K8:1171:TRP:CZ3    | 9:K8:1206:LEU:HD23   | 2.55                     | 0.41              |
| 10:C16:179:ASN:OD1   | 10:C16:213:ARG:NH1   | 2.52                     | 0.41              |
| 10:C16:271:PHE:HZ    | 10:C16:296:PHE:CZ    | 2.38                     | 0.41              |
| 10:C16:452:LEU:HG    | 10:C16:453:LEU:HG    | 2.01                     | 0.41              |
| 10:C16:855:VAL:N     | 10:C16:856:PRO:HD2   | 2.35                     | 0.41              |
| 10:C16:1764:ASN:OD1  | 10:C16:1825:LEU:HD11 | 2.20                     | 0.41              |
| 11:A24:557:LEU:CD2   | 11:A24:561:ASP:CB    | 2.90                     | 0.41              |
| 10:C24:817:HIS:HB3   | 10:C24:857:MET:SD    | 2.60                     | 0.41              |
| 10:C24:1281:THR:O    | 10:C24:1284:ASP:HB2  | 2.20                     | 0.41              |
| 10:C24:1333:HIS:ND1  | 10:C24:1337:LEU:HB2  | 2.35                     | 0.41              |
| 10:C24:1344:VAL:HG12 | 10:C24:1348:LEU:HD12 | 2.02                     | 0.41              |
| 10:C24:1624:LEU:HD22 | 10:C24:1632:LEU:CD1  | 2.50                     | 0.41              |
| 11:A40:401:GLU:HG3   | 11:A40:405:ARG:HE    | 1.85                     | 0.41              |
| 13:V:797:LEU:HD11    | 14:W:685:ILE:HG13    | 2.02                     | 0.41              |
| 14:W:718:SER:HB3     | 10:C8:1568:ARG:NH1   | 2.35                     | 0.41              |
| 10:C:31:HIS:CE1      | 10:C:35:ASN:HD21     | 2.38                     | 0.41              |
| 10:C:470:HIS:HD2     | 10:C:508:ILE:CD1     | 2.30                     | 0.41              |
| 10:C:1014:SER:O      | 10:C:1018:GLN:HG3    | 2.21                     | 0.41              |
| 10:C:1107:GLN:O      | 10:C:1110:SER:CB     | 2.67                     | 0.41              |
| 10:C:1162:PRO:C      | 10:C:1164:VAL:H      | 2.28                     | 0.41              |
| 10:C:1328:PHE:CZ     | 10:C:1377:ILE:CD1    | 2.91                     | 0.41              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 10:C:1586:VAL:HG21  | 10:C:1635:LEU:HD11   | 2.03                     | 0.41              |
| 10:C8:792:PHE:O     | 10:C8:850:ARG:NH2    | 2.54                     | 0.41              |
| 10:C8:1333:HIS:ND1  | 10:C8:1337:LEU:HB2   | 2.35                     | 0.41              |
| 11:A16:374:PHE:CE2  | 11:A16:426:ILE:HD11  | 2.54                     | 0.41              |
| 11:A16:381:TRP:NE1  | 11:A16:386:GLY:HA2   | 2.35                     | 0.41              |
| 11:A16:642:GLY:O    | 11:A16:685:ARG:HD2   | 2.19                     | 0.41              |
| 11:A32:609:ASN:OD1  | 11:A32:610:VAL:N     | 2.53                     | 0.41              |
| 11:A32:798:PHE:HZ   | 11:A32:847:ARG:NH1   | 2.02                     | 0.41              |
| 18:B:500:THR:O      | 18:B:503:SER:OG      | 2.26                     | 0.41              |
| 18:B:789:LEU:CD1    | 18:B:848:PHE:CE1     | 3.02                     | 0.41              |
| 18:B8:671:MET:HE3   | 18:B8:733:VAL:HA     | 2.00                     | 0.41              |
| 18:B8:809:THR:CG2   | 18:B8:871:ILE:CD1    | 2.98                     | 0.41              |
| 18:B8:1098:MET:CE   | 18:B8:1142:PHE:HB2   | 2.50                     | 0.41              |
| 18:B8:1154:ILE:O    | 18:B8:1158:VAL:HG23  | 2.20                     | 0.41              |
| 18:B8:1553:SER:OG   | 18:B8:1556:SER:HB3   | 2.20                     | 0.41              |
| 18:B8:1601:VAL:O    | 18:B8:1603:ASP:N     | 2.54                     | 0.41              |
| 20:E:123:CYS:HG     | 20:E:135:ILE:HD13    | 1.73                     | 0.41              |
| 20:E:261:PRO:HG2    | 20:E:301:ALA:CB      | 2.50                     | 0.41              |
| 20:E8:353:ILE:CG2   | 20:E8:413:PHE:CD2    | 2.87                     | 0.41              |
| 21:H:261:ILE:HD12   | 22:I:195:ALA:HB1     | 2.02                     | 0.41              |
| 22:I:321:LYS:HZ3    | 23:J32:711:GLU:HB2   | 1.85                     | 0.41              |
| 24:D:207:ASP:HA     | 24:D:252:VAL:HG11    | 2.03                     | 0.41              |
| 24:D:973:LEU:HD21   | 24:D:977:LYS:HE3     | 2.01                     | 0.41              |
| 24:D16:207:ASP:HA   | 24:D16:252:VAL:HG11  | 2.03                     | 0.41              |
| 10:C32:707:ILE:HD11 | 10:C32:740:LEU:HD11  | 2.02                     | 0.41              |
| 10:C32:1282:CYS:SG  | 10:C32:1347:LEU:HD13 | 2.60                     | 0.41              |
| 10:C32:1346:PHE:CD1 | 10:C32:1697:LEU:HD22 | 2.55                     | 0.41              |
| 10:C32:1708:ARG:HB2 | 10:C32:1730:ILE:CD1  | 2.50                     | 0.41              |
| 10:C32:1725:THR:C   | 10:C32:1727:SER:N    | 2.77                     | 0.41              |
| 12:A48:281:ARG:NH1  | 12:A48:381:TRP:CZ2   | 2.88                     | 0.41              |
| 12:A48:348:GLN:HB3  | 12:A48:364:ILE:HD13  | 2.02                     | 0.41              |
| 2:M:665:HIS:O       | 2:M:684:GLN:NE2      | 2.53                     | 0.41              |
| 1:R8:1229:GLU:HG3   | 1:R8:1239:TRP:O      | 2.20                     | 0.41              |
| 2:M8:641:CYS:HA     | 2:M8:644:TRP:HE1     | 1.82                     | 0.41              |
| 1:R16:1229:GLU:HG3  | 1:R16:1239:TRP:O     | 2.20                     | 0.41              |
| 2:M16:363:ARG:NH1   | 2:M16:494:SER:C      | 2.71                     | 0.41              |
| 5:P:47:ASN:ND2      | 5:P:76:LEU:O         | 2.52                     | 0.41              |
| 5:P8:105:ARG:NH2    | 5:P8:133:TYR:CB      | 2.81                     | 0.41              |
| 5:P8:214:LEU:HD12   | 5:P8:245:TRP:HZ3     | 1.86                     | 0.41              |
| 7:Q8:102:ALA:HB1    | 7:Q8:137:VAL:HB      | 2.02                     | 0.41              |
| 7:Q8:236:HIS:ND1    | 7:Q8:237:PRO:HD2     | 2.36                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 7:Q16:102:ALA:HB1    | 7:Q16:137:VAL:HB     | 2.02                     | 0.41              |
| 7:Q16:172:LYS:HD3    | 7:Q16:175:ASP:HB2    | 2.02                     | 0.41              |
| 8:L8:608:PHE:CD2     | 8:L8:635:MET:HG2     | 2.55                     | 0.41              |
| 9:K:926:ILE:HD11     | 9:K:937:ILE:HD11     | 2.02                     | 0.41              |
| 9:K:1117:LEU:HG      | 9:K:1139:ILE:CD1     | 2.38                     | 0.41              |
| 9:K:1281:SER:O       | 9:K:1283:PRO:HD3     | 2.21                     | 0.41              |
| 9:K8:736:LEU:HD21    | 9:K8:770:VAL:HG13    | 2.02                     | 0.41              |
| 10:C16:50:LYS:HA     | 10:C16:51:PRO:HD3    | 1.94                     | 0.41              |
| 10:C16:234:VAL:HG21  | 10:C16:286:ILE:CD1   | 2.50                     | 0.41              |
| 10:C16:265:PHE:O     | 10:C16:269:ILE:HG13  | 2.20                     | 0.41              |
| 10:C16:300:VAL:HG12  | 10:C16:317:ARG:HG2   | 1.99                     | 0.41              |
| 10:C16:707:ILE:HD11  | 10:C16:740:LEU:HD11  | 2.02                     | 0.41              |
| 10:C16:1344:VAL:HG12 | 10:C16:1348:LEU:HD12 | 2.02                     | 0.41              |
| 10:C16:1346:PHE:CD1  | 10:C16:1697:LEU:HD22 | 2.55                     | 0.41              |
| 10:C16:1389:ILE:HD12 | 10:C16:1426:ARG:NH1  | 2.23                     | 0.41              |
| 10:C16:1442:GLN:O    | 10:C16:1444:GLY:N    | 2.49                     | 0.41              |
| 11:A24:156:MET:CG    | 11:A24:555:HIS:CE1   | 2.81                     | 0.41              |
| 10:C24:33:ILE:HG21   | 10:C24:158:LEU:HD22  | 2.02                     | 0.41              |
| 10:C24:962:PHE:HZ    | 10:C24:997:ILE:CD1   | 2.17                     | 0.41              |
| 10:C24:988:GLN:HE21  | 10:C24:1064:PHE:HE1  | 1.59                     | 0.41              |
| 10:C24:1764:ASN:OD1  | 10:C24:1825:LEU:HD11 | 2.20                     | 0.41              |
| 11:A40:823:VAL:O     | 11:A40:830:ILE:HD13  | 2.20                     | 0.41              |
| 13:V:797:LEU:HD11    | 14:W:685:ILE:CG1     | 2.50                     | 0.41              |
| 15:J:680:LEU:O       | 15:J:681:GLU:C       | 2.57                     | 0.41              |
| 10:C:265:PHE:O       | 10:C:269:ILE:HG13    | 2.20                     | 0.41              |
| 10:C:1333:HIS:ND1    | 10:C:1337:LEU:HB2    | 2.35                     | 0.41              |
| 10:C:1708:ARG:HB2    | 10:C:1730:ILE:CD1    | 2.50                     | 0.41              |
| 10:C8:1014:SER:O     | 10:C8:1018:GLN:HG3   | 2.20                     | 0.41              |
| 10:C8:1219:ILE:CD1   | 10:C8:1229:LEU:HD21  | 2.50                     | 0.41              |
| 10:C8:1263:LYS:HD3   | 10:C8:1263:LYS:HA    | 1.87                     | 0.41              |
| 10:C8:1290:HIS:CB    | 10:C8:1334:MET:CE    | 2.73                     | 0.41              |
| 10:C8:1624:LEU:HD22  | 10:C8:1632:LEU:CD1   | 2.50                     | 0.41              |
| 10:C8:1708:ARG:HB2   | 10:C8:1730:ILE:CD1   | 2.50                     | 0.41              |
| 11:A32:374:PHE:CE2   | 11:A32:426:ILE:HD11  | 2.54                     | 0.41              |
| 11:A32:714:GLY:CA    | 24:D32:1398:ARG:CZ   | 2.84                     | 0.41              |
| 17:F16:69:SER:HA     | 17:F16:70:PRO:HD3    | 1.82                     | 0.41              |
| 18:B:409:LEU:O       | 18:B:462:ARG:NH2     | 2.53                     | 0.41              |
| 18:B:413:ASP:C       | 18:B:415:THR:H       | 2.28                     | 0.41              |
| 18:B:955:VAL:HG13    | 18:B:959:PHE:HD2     | 1.86                     | 0.41              |
| 18:B:1700:LEU:CD2    | 18:B:1833:PHE:CE2    | 3.03                     | 0.41              |
| 18:B:1745:HIS:C      | 18:B:1747:SER:N      | 2.76                     | 0.41              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B8:955:VAL:HG13  | 18:B8:959:PHE:HD2    | 1.86                     | 0.41              |
| 20:E:414:MET:HE2    | 20:E:455:TYR:CE2     | 2.55                     | 0.41              |
| 21:H:156:GLU:HA     | 21:H:157:PRO:HD3     | 1.87                     | 0.41              |
| 21:H:284:LEU:C      | 23:J32:650:GLN:NE2   | 2.77                     | 0.41              |
| 23:J16:686:MET:CE   | 23:J16:694:ARG:HH21  | 2.10                     | 0.41              |
| 10:C32:31:HIS:CE1   | 10:C32:35:ASN:HD21   | 2.38                     | 0.41              |
| 10:C32:919:ASP:H    | 10:C32:927:THR:HG23  | 1.84                     | 0.41              |
| 10:C32:1314:GLU:OE1 | 10:C32:1396:SER:OG   | 2.38                     | 0.41              |
| 10:C32:1812:GLU:CG  | 10:C32:1819:LEU:HD12 | 2.50                     | 0.41              |
| 12:A48:650:GLY:HA2  | 12:A48:659:ARG:NH2   | 2.36                     | 0.41              |
| 2:M:714:GLU:HA      | 2:M:714:GLU:OE2      | 2.21                     | 0.41              |
| 1:R8:983:ARG:HD3    | 24:D40:1364:PRO:HA   | 2.03                     | 0.41              |
| 2:M8:625:HIS:NE2    | 3:N8:225:PRO:HB3     | 2.34                     | 0.41              |
| 2:M8:691:TRP:CE2    | 2:M8:725:ARG:HG3     | 2.55                     | 0.41              |
| 1:R16:341:ARG:HH12  | 1:R16:499:GLU:CD     | 2.28                     | 0.41              |
| 2:M16:624:ASP:OD1   | 2:M16:624:ASP:N      | 2.51                     | 0.41              |
| 2:M16:714:GLU:OE2   | 2:M16:714:GLU:HA     | 2.21                     | 0.41              |
| 5:P16:566:PHE:CZ    | 5:P16:597:GLY:O      | 2.71                     | 0.41              |
| 6:O16:61:LYS:CE     | 6:O16:112:ASP:OD1    | 2.63                     | 0.41              |
| 6:O16:179:LYS:CE    | 6:O16:183:GLN:OE1    | 2.56                     | 0.41              |
| 7:Q16:254:ALA:HB3   | 7:Q16:302:ILE:CD1    | 2.50                     | 0.41              |
| 9:K8:585:GLU:CA     | 9:K8:622:VAL:HG13    | 2.49                     | 0.41              |
| 9:K8:1025:TRP:CH2   | 9:K8:1026:LEU:HD12   | 2.56                     | 0.41              |
| 9:K16:1180:TRP:CZ2  | 9:K16:1206:LEU:HD12  | 2.55                     | 0.41              |
| 10:C16:696:GLN:OE1  | 10:C16:783:LEU:HD11  | 2.21                     | 0.41              |
| 10:C16:1163:LEU:C   | 10:C16:1166:SER:H    | 2.28                     | 0.41              |
| 11:A24:374:PHE:CE2  | 11:A24:426:ILE:HD11  | 2.54                     | 0.41              |
| 11:A24:567:SER:OG   | 11:A24:619:MET:HE1   | 2.21                     | 0.41              |
| 10:C24:267:LEU:CD1  | 10:C24:316:ILE:HD12  | 2.51                     | 0.41              |
| 10:C24:1062:GLU:HA  | 10:C24:1063:PRO:HD3  | 1.68                     | 0.41              |
| 11:A40:212:LYS:HE3  | 11:A40:585:MET:HE3   | 1.76                     | 0.41              |
| 13:V:754:PHE:O      | 13:V:758:CYS:HB2     | 2.19                     | 0.41              |
| 14:W:715:ASP:CA     | 10:C8:1568:ARG:CZ    | 2.77                     | 0.41              |
| 10:C:148:GLU:HA     | 10:C:149:PRO:HD3     | 1.79                     | 0.41              |
| 10:C:234:VAL:HG21   | 10:C:286:ILE:CD1     | 2.50                     | 0.41              |
| 10:C:615:GLU:CA     | 10:C:619:LEU:HD12    | 2.49                     | 0.41              |
| 10:C:919:ASP:H      | 10:C:927:THR:HG23    | 1.84                     | 0.41              |
| 10:C:1043:ALA:O     | 10:C:1047:ILE:HG13   | 2.21                     | 0.41              |
| 10:C:1385:LEU:HD11  | 10:C:1419:PHE:CD1    | 2.56                     | 0.41              |
| 10:C:1593:TRP:CE2   | 10:C:1603:PHE:HD2    | 2.37                     | 0.41              |
| 10:C:1616:ILE:O     | 10:C:1618:SER:N      | 2.46                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:1764:ASN:OD1   | 10:C:1825:LEU:HD11  | 2.20                     | 0.41              |
| 10:C8:148:GLU:HA    | 10:C8:149:PRO:HD3   | 1.79                     | 0.41              |
| 10:C8:271:PHE:HZ    | 10:C8:296:PHE:CZ    | 2.38                     | 0.41              |
| 10:C8:275:ALA:CB    | 10:C8:326:LEU:CD1   | 2.96                     | 0.41              |
| 10:C8:277:SER:O     | 10:C8:280:SER:N     | 2.36                     | 0.41              |
| 10:C8:300:VAL:HG12  | 10:C8:317:ARG:HG2   | 1.99                     | 0.41              |
| 10:C8:817:HIS:HB3   | 10:C8:857:MET:SD    | 2.60                     | 0.41              |
| 10:C8:1250:ALA:HB2  | 10:C8:1309:ARG:HH11 | 1.78                     | 0.41              |
| 10:C8:1812:GLU:CG   | 10:C8:1819:LEU:HD12 | 2.50                     | 0.41              |
| 10:C8:1832:MET:HE2  | 10:C8:1832:MET:HB2  | 1.66                     | 0.41              |
| 11:A32:381:TRP:NE1  | 11:A32:386:GLY:HA2  | 2.36                     | 0.41              |
| 11:A32:631:GLU:O    | 11:A32:632:ARG:HB2  | 2.20                     | 0.41              |
| 18:B:90:ILE:HD11    | 18:B:131:ILE:HD12   | 2.02                     | 0.41              |
| 18:B:1439:LYS:HG2   | 18:B:1500:LEU:CD1   | 2.40                     | 0.41              |
| 18:B8:34:GLN:N      | 18:B8:35:PRO:HD2    | 2.34                     | 0.41              |
| 18:B8:216:ASP:OD1   | 18:B8:270:GLN:NE2   | 2.53                     | 0.41              |
| 18:B8:313:ILE:CD1   | 18:B8:331:TRP:CE3   | 3.02                     | 0.41              |
| 18:B8:489:LYS:O     | 18:B8:491:VAL:HG22  | 2.21                     | 0.41              |
| 18:B8:612:GLY:O     | 18:B8:614:MET:N     | 2.51                     | 0.41              |
| 18:B8:809:THR:HG23  | 18:B8:871:ILE:CD1   | 2.50                     | 0.41              |
| 18:B8:809:THR:HG23  | 18:B8:871:ILE:HD12  | 2.02                     | 0.41              |
| 18:B8:1375:SER:O    | 18:B8:1379:VAL:HG23 | 2.20                     | 0.41              |
| 18:B8:1456:ASN:OD1  | 18:B8:1510:TYR:CD1  | 2.73                     | 0.41              |
| 20:E:206:GLY:O      | 20:E:208:VAL:N      | 2.46                     | 0.41              |
| 19:48:220:TRP:CD2   | 19:48:227:LEU:HD13  | 2.56                     | 0.41              |
| 19:48:421:GLN:HB3   | 19:48:440:ILE:HG23  | 2.01                     | 0.41              |
| 20:E8:21:TRP:O      | 20:E8:25:PRO:HD2    | 2.21                     | 0.41              |
| 20:E8:148:VAL:O     | 20:E8:152:THR:HG23  | 2.20                     | 0.41              |
| 20:E8:201:LEU:C     | 20:E8:203:TRP:N     | 2.77                     | 0.41              |
| 20:E8:261:PRO:HG2   | 20:E8:301:ALA:CB    | 2.50                     | 0.41              |
| 21:H:288:THR:CB     | 23:J32:650:GLN:NE2  | 2.75                     | 0.41              |
| 21:H:316:ILE:O      | 21:H:316:ILE:CG2    | 2.65                     | 0.41              |
| 22:I8:321:LYS:NZ    | 23:J8:711:GLU:HB2   | 2.35                     | 0.41              |
| 21:H24:190:TRP:HA   | 21:H24:191:PRO:HD3  | 1.89                     | 0.41              |
| 21:H24:288:THR:CB   | 23:J24:650:GLN:NE2  | 2.75                     | 0.41              |
| 24:D40:1284:ILE:CD1 | 24:D40:1319:ALA:HA  | 2.51                     | 0.41              |
| 10:C32:234:VAL:HG21 | 10:C32:286:ILE:CD1  | 2.50                     | 0.41              |
| 10:C32:259:ILE:O    | 10:C32:262:SER:OG   | 2.35                     | 0.41              |
| 10:C32:267:LEU:CD1  | 10:C32:316:ILE:HD12 | 2.51                     | 0.41              |
| 10:C32:821:ILE:HD11 | 10:C32:861:ILE:HD13 | 2.03                     | 0.41              |
| 10:C32:879:LEU:CD2  | 10:C32:944:MET:HG3  | 2.49                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C32:994:LEU:HD11  | 10:C32:1026:LEU:CD1  | 2.51                     | 0.41              |
| 10:C32:1014:SER:O    | 10:C32:1018:GLN:HG3  | 2.20                     | 0.41              |
| 10:C32:1344:VAL:HG12 | 10:C32:1348:LEU:HD12 | 2.02                     | 0.41              |
| 10:C32:1586:VAL:HG21 | 10:C32:1635:LEU:HD11 | 2.03                     | 0.41              |
| 12:A48:763:HIS:CE1   | 12:A48:815:VAL:HG21  | 2.55                     | 0.41              |
| 2:M:503:TYR:HE1      | 2:M:507:LEU:HD11     | 1.85                     | 0.41              |
| 2:M:565:THR:HG21     | 2:M:570:ASP:OD2      | 2.21                     | 0.41              |
| 2:M:625:HIS:CB       | 3:N:165:GLY:HA2      | 2.51                     | 0.41              |
| 1:R8:1180:PRO:HB3    | 1:R8:1211:LYS:HB3    | 2.02                     | 0.41              |
| 2:M8:843:ALA:O       | 4:T8:656:TRP:HH2     | 2.03                     | 0.41              |
| 1:R16:1168:LEU:HD23  | 1:R16:1216:ILE:HG12  | 2.02                     | 0.41              |
| 2:M16:443:ARG:HG2    | 2:M16:448:ASP:OD2    | 2.20                     | 0.41              |
| 5:P:251:LYS:CE       | 14:W:765:LYS:NZ      | 2.84                     | 0.41              |
| 5:P:633:LEU:HD23     | 5:P:633:LEU:O        | 2.20                     | 0.41              |
| 7:Q:32:ASN:HB3       | 7:Q:34:PHE:CZ        | 2.55                     | 0.41              |
| 5:P8:55:ARG:HH22     | 5:P8:62:ASP:HB2      | 1.85                     | 0.41              |
| 5:P8:682:ARG:HG3     | 5:P8:687:PHE:CE1     | 2.56                     | 0.41              |
| 7:Q8:32:ASN:HB3      | 7:Q8:34:PHE:CZ       | 2.55                     | 0.41              |
| 5:P16:112:LEU:HB3    | 5:P16:123:GLN:HE21   | 1.86                     | 0.41              |
| 5:P16:143:ASN:C      | 5:P16:145:ILE:N      | 2.78                     | 0.41              |
| 5:P16:233:TYR:CZ     | 5:P16:237:MET:CE     | 3.03                     | 0.41              |
| 6:O16:286:MET:HB3    | 6:O16:295:LEU:HD11   | 2.01                     | 0.41              |
| 8:L16:173:ASP:CG     | 12:A48:783:PHE:CE1   | 2.98                     | 0.41              |
| 9:K:792:LEU:CG       | 9:K:864:ILE:CD1      | 2.75                     | 0.41              |
| 9:K:1039:ASP:OD1     | 9:K:1096:LYS:CE      | 2.67                     | 0.41              |
| 9:K:1150:GLU:OE1     | 9:K:1212:ARG:CZ      | 2.68                     | 0.41              |
| 10:C16:456:ASN:C     | 10:C16:458:VAL:N     | 2.76                     | 0.41              |
| 10:C16:1280:VAL:HA   | 10:C16:1731:HIS:HE1  | 1.85                     | 0.41              |
| 10:C24:271:PHE:HZ    | 10:C24:296:PHE:CZ    | 2.38                     | 0.41              |
| 10:C24:879:LEU:CD2   | 10:C24:944:MET:HG3   | 2.50                     | 0.41              |
| 10:C24:1014:SER:O    | 10:C24:1018:GLN:HG3  | 2.20                     | 0.41              |
| 10:C24:1162:PRO:C    | 10:C24:1164:VAL:H    | 2.28                     | 0.41              |
| 10:C24:1708:ARG:HB2  | 10:C24:1730:ILE:CD1  | 2.50                     | 0.41              |
| 11:A40:156:MET:HE2   | 11:A40:555:HIS:HD1   | 1.75                     | 0.41              |
| 11:A40:426:ILE:O     | 11:A40:459:ARG:NH2   | 2.54                     | 0.41              |
| 12:A:401:GLU:HG3     | 12:A:405:ARG:HE      | 1.85                     | 0.41              |
| 12:A:631:GLU:O       | 12:A:632:ARG:HB2     | 2.21                     | 0.41              |
| 12:A:849:TRP:HB2     | 12:A:854:TYR:CE2     | 2.54                     | 0.41              |
| 13:V:836:LEU:CD2     | 14:W:716:PHE:HE1     | 2.33                     | 0.41              |
| 14:W:628:HIS:HA      | 14:W:632:ILE:HD12    | 2.02                     | 0.41              |
| 10:C:456:ASN:C       | 10:C:458:VAL:N       | 2.76                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C:994:LEU:HD11    | 10:C:1026:LEU:CD1    | 2.51                     | 0.41              |
| 10:C:1442:GLN:O      | 10:C:1444:GLY:N      | 2.49                     | 0.41              |
| 10:C:1832:MET:HE2    | 10:C:1832:MET:HB2    | 1.66                     | 0.41              |
| 10:C8:320:TRP:NE1    | 10:C8:324:LEU:HD11   | 2.36                     | 0.41              |
| 10:C8:960:PHE:CE2    | 10:C8:1138:GLU:OE2   | 2.71                     | 0.41              |
| 10:C8:1280:VAL:HA    | 10:C8:1731:HIS:HE1   | 1.85                     | 0.41              |
| 10:C8:1309:ARG:NE    | 10:C8:1311:GLU:O     | 2.53                     | 0.41              |
| 10:C8:1442:GLN:O     | 10:C8:1444:GLY:N     | 2.49                     | 0.41              |
| 11:A16:567:SER:OG    | 11:A16:619:MET:HE1   | 2.21                     | 0.41              |
| 11:A32:98:ALA:O      | 18:B8:1103:LYS:CE    | 2.68                     | 0.41              |
| 11:A32:790:MET:O     | 11:A32:836:LYS:NZ    | 2.49                     | 0.41              |
| 18:B:216:ASP:OD1     | 18:B:270:GLN:NE2     | 2.53                     | 0.41              |
| 18:B:467:ILE:HD11    | 18:B:559:LEU:CD1     | 2.50                     | 0.41              |
| 18:B:489:LYS:O       | 18:B:491:VAL:HG22    | 2.21                     | 0.41              |
| 18:B:628:VAL:HA      | 18:B:631:LEU:CD1     | 2.50                     | 0.41              |
| 18:B:809:THR:HG23    | 18:B:871:ILE:CD1     | 2.50                     | 0.41              |
| 18:B:1661:TYR:CE1    | 18:B:1689:TYR:HE2    | 2.39                     | 0.41              |
| 18:B8:413:ASP:C      | 18:B8:415:THR:H      | 2.28                     | 0.41              |
| 18:B8:1865:LEU:O     | 18:B8:1869:GLN:HG3   | 2.21                     | 0.41              |
| 19:4:31:GLN:OE1      | 19:4:41:VAL:HG23     | 2.20                     | 0.41              |
| 19:4:38:LEU:HD11     | 19:4:438:PRO:HB3     | 2.02                     | 0.41              |
| 20:E:21:TRP:O        | 20:E:25:PRO:HD2      | 2.21                     | 0.41              |
| 20:E:208:VAL:HG12    | 20:E:212:LYS:HB3     | 2.03                     | 0.41              |
| 19:48:103:GLN:NE2    | 19:48:411:LEU:CD1    | 2.75                     | 0.41              |
| 19:48:125:ILE:HD11   | 19:48:139:LEU:HD11   | 2.02                     | 0.41              |
| 20:E8:175:LEU:HB2    | 20:E8:176:PRO:HD3    | 2.02                     | 0.41              |
| 20:E8:347:PRO:C      | 20:E8:349:THR:N      | 2.78                     | 0.41              |
| 22:I:97:THR:HG22     | 22:I:107:THR:CG2     | 2.48                     | 0.41              |
| 22:I24:321:LYS:HZ3   | 23:J24:711:GLU:HB2   | 1.85                     | 0.41              |
| 24:D8:243:VAL:HA     | 24:D8:244:PRO:HD3    | 1.93                     | 0.41              |
| 10:C32:572:ILE:CG1   | 10:C32:606:MET:CE    | 2.90                     | 0.41              |
| 10:C32:878:ARG:NH2   | 10:C32:885:VAL:CG2   | 2.69                     | 0.41              |
| 10:C32:1219:ILE:CD1  | 10:C32:1229:LEU:HD21 | 2.50                     | 0.41              |
| 10:C32:1385:LEU:HD11 | 10:C32:1419:PHE:CD1  | 2.56                     | 0.41              |
| 10:C32:1502:ARG:O    | 10:C32:1504:ASP:N    | 2.53                     | 0.41              |
| 1:R:771:SER:CB       | 24:D:1317:ARG:CD     | 2.88                     | 0.41              |
| 2:M:162:ILE:CD1      | 2:M:213:LEU:CD1      | 2.97                     | 0.41              |
| 3:N:301:GLU:HA       | 3:N:302:PRO:HD3      | 1.91                     | 0.41              |
| 2:M8:187:PHE:HA      | 3:N8:15:HIS:O        | 2.21                     | 0.41              |
| 2:M8:417:ARG:CZ      | 8:L8:415:PHE:HZ      | 2.27                     | 0.41              |
| 2:M16:198:PHE:CE1    | 2:M16:219:LYS:HG3    | 2.55                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:M16:810:LEU:CD2    | 2:M16:819:GLN:HA     | 2.51                     | 0.41              |
| 3:N16:4:GLN:NE2      | 3:N16:44:GLY:HA3     | 2.27                     | 0.41              |
| 3:N16:169:SER:O      | 3:N16:170:SER:C      | 2.62                     | 0.41              |
| 4:T:671:ILE:HG21     | 5:P:699:SER:HA       | 2.02                     | 0.41              |
| 5:P:325:PHE:CG       | 13:V:771:GLN:NE2     | 2.89                     | 0.41              |
| 5:P:566:PHE:HE1      | 5:P:600:PHE:HD1      | 1.68                     | 0.41              |
| 7:Q:254:ALA:HB3      | 7:Q:302:ILE:CD1      | 2.50                     | 0.41              |
| 6:O8:17:TRP:CE2      | 6:O8:24:LEU:HD13     | 2.55                     | 0.41              |
| 6:O8:82:LEU:CD2      | 6:O8:103:MET:HE1     | 2.48                     | 0.41              |
| 7:Q16:236:HIS:NE2    | 7:Q16:303:LEU:CD1    | 2.83                     | 0.41              |
| 9:K:798:LEU:HB3      | 9:K:842:ILE:CD1      | 2.51                     | 0.41              |
| 9:K:971:LEU:O        | 9:K:975:MET:HG3      | 2.20                     | 0.41              |
| 9:K8:751:LEU:HD23    | 9:K8:754:ARG:HD3     | 1.98                     | 0.41              |
| 10:C16:62:ILE:CD1    | 10:C16:95:VAL:HG21   | 2.51                     | 0.41              |
| 10:C16:97:LEU:HD21   | 10:C16:123:TRP:HB2   | 2.03                     | 0.41              |
| 10:C16:847:ARG:CD    | 10:C16:903:ASN:CG    | 2.94                     | 0.41              |
| 10:C16:1043:ALA:O    | 10:C16:1047:ILE:HG13 | 2.21                     | 0.41              |
| 10:C16:1162:PRO:C    | 10:C16:1164:VAL:H    | 2.28                     | 0.41              |
| 10:C16:1280:VAL:CG2  | 10:C16:1731:HIS:CE1  | 2.95                     | 0.41              |
| 10:C16:1624:LEU:HD22 | 10:C16:1632:LEU:CD1  | 2.50                     | 0.41              |
| 11:A24:803:PRO:CG    | 24:D8:1401:LEU:HD12  | 2.41                     | 0.41              |
| 10:C24:698:PHE:CZ    | 10:C24:749:LEU:CD1   | 3.02                     | 0.41              |
| 10:C24:847:ARG:CD    | 10:C24:903:ASN:CG    | 2.94                     | 0.41              |
| 10:C24:994:LEU:HD11  | 10:C24:1026:LEU:CD1  | 2.51                     | 0.41              |
| 10:C24:1163:LEU:C    | 10:C24:1166:SER:H    | 2.28                     | 0.41              |
| 10:C24:1283:LEU:CD1  | 10:C24:1357:LEU:HD13 | 2.49                     | 0.41              |
| 10:C24:1309:ARG:NE   | 10:C24:1311:GLU:O    | 2.53                     | 0.41              |
| 10:C24:1314:GLU:OE1  | 10:C24:1396:SER:OG   | 2.38                     | 0.41              |
| 11:A40:10:TRP:HH2    | 21:H16:338:MET:HE3   | 1.85                     | 0.41              |
| 11:A40:56:ALA:O      | 11:A40:58:SER:N      | 2.54                     | 0.41              |
| 11:A40:232:ASP:O     | 11:A40:236:THR:HG23  | 2.20                     | 0.41              |
| 12:A:259:ILE:HG23    | 12:A:276:LEU:CD2     | 2.51                     | 0.41              |
| 13:V:861:PHE:CZ      | 14:W:742:VAL:CG2     | 3.03                     | 0.41              |
| 14:W:236:THR:HG23    | 14:W:248:ILE:HG23    | 2.02                     | 0.41              |
| 10:C:97:LEU:HD21     | 10:C:123:TRP:HB2     | 2.02                     | 0.41              |
| 10:C8:821:ILE:HD11   | 10:C8:861:ILE:HD13   | 2.03                     | 0.41              |
| 10:C8:1105:LEU:HD21  | 10:C8:1183:LEU:HD21  | 2.01                     | 0.41              |
| 11:A32:56:ALA:O      | 11:A32:58:SER:N      | 2.54                     | 0.41              |
| 17:F16:74:ILE:HG22   | 17:F16:76:ASP:H      | 1.86                     | 0.41              |
| 18:B:586:VAL:HB      | 18:B:593:CYS:SG      | 2.61                     | 0.41              |
| 18:B:809:THR:CG2     | 18:B:871:ILE:CD1     | 2.98                     | 0.41              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 18:B:1098:MET:CE    | 18:B:1142:PHE:CB     | 2.99                     | 0.41              |
| 18:B:1363:ALA:O     | 18:B:1365:ARG:N      | 2.53                     | 0.41              |
| 18:B:1601:VAL:O     | 18:B:1603:ASP:N      | 2.53                     | 0.41              |
| 18:B:1676:VAL:O     | 18:B:1676:VAL:HG12   | 2.21                     | 0.41              |
| 18:B:1793:ILE:O     | 18:B:1793:ILE:HG22   | 2.20                     | 0.41              |
| 18:B8:90:ILE:HD11   | 18:B8:131:ILE:HD12   | 2.02                     | 0.41              |
| 18:B8:786:ASP:OD2   | 24:D32:1066:VAL:CG1  | 2.49                     | 0.41              |
| 18:B8:886:ASN:HA    | 18:B8:887:PRO:HD2    | 1.98                     | 0.41              |
| 18:B8:1072:LEU:CD2  | 18:B8:1076:GLU:OE2   | 2.56                     | 0.41              |
| 18:B8:1101:TYR:CZ   | 18:B8:1105:LEU:HD11  | 2.54                     | 0.41              |
| 18:B8:1363:ALA:O    | 18:B8:1365:ARG:N     | 2.53                     | 0.41              |
| 18:B8:1745:HIS:C    | 18:B8:1747:SER:N     | 2.76                     | 0.41              |
| 19:4:253:GLY:HA3    | 19:4:273:ARG:NH2     | 2.36                     | 0.41              |
| 20:E8:84:GLY:HA3    | 20:E8:94:PHE:CZ      | 2.56                     | 0.41              |
| 21:H:291:VAL:HG11   | 23:J32:657:GLU:CG    | 2.46                     | 0.41              |
| 21:H:312:GLN:NE2    | 22:I:290:ASP:HB3     | 2.16                     | 0.41              |
| 21:H24:193:LEU:CD2  | 21:H24:195:GLN:HE21  | 2.18                     | 0.41              |
| 21:H24:231:HIS:CG   | 23:J24:596:GLN:HE22  | 2.31                     | 0.41              |
| 22:I24:307:VAL:O    | 22:I24:311:VAL:HG23  | 2.20                     | 0.41              |
| 24:D:313:VAL:HG21   | 24:D16:13:THR:HG21   | 2.03                     | 0.41              |
| 24:D:1099:ARG:CZ    | 24:D:1149:VAL:HG11   | 2.51                     | 0.41              |
| 24:D32:207:ASP:HA   | 24:D32:252:VAL:HG11  | 2.03                     | 0.41              |
| 24:D32:749:ARG:HH22 | 24:D40:397:ALA:CB    | 2.32                     | 0.41              |
| 10:C32:271:PHE:HZ   | 10:C32:296:PHE:CZ    | 2.38                     | 0.41              |
| 10:C32:562:PRO:HA   | 10:C32:565:ARG:CD    | 2.49                     | 0.41              |
| 10:C32:847:ARG:CD   | 10:C32:903:ASN:CG    | 2.94                     | 0.41              |
| 10:C32:855:VAL:N    | 10:C32:856:PRO:HD2   | 2.35                     | 0.41              |
| 10:C32:1162:PRO:C   | 10:C32:1164:VAL:H    | 2.28                     | 0.41              |
| 10:C32:1764:ASN:OD1 | 10:C32:1825:LEU:HD11 | 2.20                     | 0.41              |
| 1:R:1242:SER:HG     | 1:R:1244:LEU:HD12    | 1.84                     | 0.41              |
| 2:M:236:GLN:OE1     | 2:M:297:VAL:CG1      | 2.68                     | 0.41              |
| 2:M:544:LEU:CD2     | 2:M:581:LEU:HD22     | 2.51                     | 0.41              |
| 2:M:813:ASN:HA      | 2:M:814:PRO:HD3      | 1.83                     | 0.41              |
| 1:R8:638:ILE:HD12   | 1:R8:638:ILE:HA      | 1.93                     | 0.41              |
| 1:R8:672:LYS:HZ2    | 1:R8:842:ASP:CG      | 2.28                     | 0.41              |
| 1:R8:1188:TYR:CZ    | 24:D40:1459:LEU:CD1  | 3.04                     | 0.41              |
| 2:M8:202:LYS:CE     | 2:M8:208:SER:O       | 2.61                     | 0.41              |
| 2:M8:447:LEU:HD21   | 8:L8:280:GLN:NE2     | 2.35                     | 0.41              |
| 2:M8:714:GLU:OE2    | 2:M8:714:GLU:HA      | 2.21                     | 0.41              |
| 2:M8:810:LEU:CD2    | 2:M8:819:GLN:HA      | 2.51                     | 0.41              |
| 1:R16:1248:PRO:C    | 1:R16:1250:ASP:H     | 2.28                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P:682:ARG:HG3      | 5:P:687:PHE:CE1      | 2.56                     | 0.41              |
| 6:O:82:LEU:HD23      | 6:O:103:MET:HE1      | 1.87                     | 0.41              |
| 6:O:286:MET:HB3      | 6:O:295:LEU:HD11     | 2.01                     | 0.41              |
| 7:Q:314:LEU:CD2      | 7:Q:327:LEU:HD12     | 2.51                     | 0.41              |
| 5:P8:16:PHE:HE1      | 6:O8:311:LEU:HD21    | 1.82                     | 0.41              |
| 6:O8:236:PRO:O       | 6:O8:240:ARG:NH2     | 2.49                     | 0.41              |
| 7:Q16:314:LEU:CD2    | 7:Q16:327:LEU:HD12   | 2.51                     | 0.41              |
| 8:L16:1069:LEU:CD1   | 9:K16:1086:VAL:CG1   | 2.66                     | 0.41              |
| 9:K:1048:GLN:HE22    | 9:K:1128:ARG:CA      | 2.34                     | 0.41              |
| 9:K8:786:GLN:HE22    | 9:K8:794:ARG:HH11    | 1.66                     | 0.41              |
| 9:K8:798:LEU:HB3     | 9:K8:842:ILE:CD1     | 2.51                     | 0.41              |
| 9:K8:1222:PHE:CD2    | 9:K8:1223:ASP:HB2    | 2.56                     | 0.41              |
| 10:C16:267:LEU:CD1   | 10:C16:316:ILE:HD12  | 2.51                     | 0.41              |
| 10:C16:615:GLU:C     | 10:C16:619:LEU:HD12  | 2.45                     | 0.41              |
| 10:C16:817:HIS:HB3   | 10:C16:857:MET:SD    | 2.60                     | 0.41              |
| 10:C16:1385:LEU:HD11 | 10:C16:1419:PHE:CD1  | 2.56                     | 0.41              |
| 10:C16:1586:VAL:HG21 | 10:C16:1635:LEU:HD11 | 2.02                     | 0.41              |
| 10:C16:1812:GLU:CG   | 10:C16:1819:LEU:HD12 | 2.50                     | 0.41              |
| 11:A24:232:ASP:O     | 11:A24:236:THR:HG23  | 2.20                     | 0.41              |
| 11:A24:381:TRP:NE1   | 11:A24:386:GLY:HA2   | 2.36                     | 0.41              |
| 11:A24:426:ILE:O     | 11:A24:459:ARG:NH2   | 2.54                     | 0.41              |
| 11:A24:631:GLU:O     | 11:A24:632:ARG:HB2   | 2.20                     | 0.41              |
| 10:C24:97:LEU:HD21   | 10:C24:123:TRP:HB2   | 2.03                     | 0.41              |
| 10:C24:707:ILE:HD11  | 10:C24:740:LEU:HD11  | 2.02                     | 0.41              |
| 10:C24:1043:ALA:O    | 10:C24:1047:ILE:HG13 | 2.21                     | 0.41              |
| 11:A40:704:ILE:HG12  | 11:A40:760:LEU:CD1   | 2.49                     | 0.41              |
| 11:A40:794:THR:C     | 11:A40:796:ASP:N     | 2.77                     | 0.41              |
| 12:A:232:ASP:O       | 12:A:236:THR:HG23    | 2.20                     | 0.41              |
| 12:A:798:PHE:HZ      | 12:A:847:ARG:NH1     | 2.01                     | 0.41              |
| 10:C:817:HIS:HB3     | 10:C:857:MET:SD      | 2.60                     | 0.41              |
| 10:C:837:ARG:CZ      | 10:C:890:ASP:CB      | 2.92                     | 0.41              |
| 10:C:847:ARG:CD      | 10:C:903:ASN:CG      | 2.94                     | 0.41              |
| 10:C:1127:THR:O      | 10:C:1128:SER:C      | 2.62                     | 0.41              |
| 10:C8:97:LEU:HD21    | 10:C8:123:TRP:HB2    | 2.02                     | 0.41              |
| 10:C8:879:LEU:CD2    | 10:C8:944:MET:HG3    | 2.50                     | 0.41              |
| 10:C8:1507:LEU:C     | 10:C8:1509:SER:N     | 2.67                     | 0.41              |
| 11:A16:10:TRP:HH2    | 21:H:338:MET:HE3     | 1.85                     | 0.41              |
| 11:A16:121:GLN:NE2   | 18:B:1559:ALA:CA     | 2.52                     | 0.41              |
| 11:A16:631:GLU:O     | 11:A16:632:ARG:HB2   | 2.20                     | 0.41              |
| 11:A16:696:ILE:HD13  | 11:A16:725:GLY:N     | 2.36                     | 0.41              |
| 11:A32:567:SER:OG    | 11:A32:619:MET:HE1   | 2.21                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A32:823:VAL:O     | 11:A32:830:ILE:HD13  | 2.20                     | 0.41              |
| 18:B:603:PHE:HB3     | 18:B:619:ARG:HH22    | 1.84                     | 0.41              |
| 18:B:671:MET:HE3     | 18:B:733:VAL:HA      | 2.00                     | 0.41              |
| 18:B:938:LEU:HD11    | 18:B:1005:TYR:CE1    | 2.55                     | 0.41              |
| 18:B:1418:ALA:HB3    | 18:B:1422:LEU:HD12   | 2.02                     | 0.41              |
| 18:B:1518:VAL:O      | 18:B:1522:LEU:HG     | 2.21                     | 0.41              |
| 18:B:1865:LEU:O      | 18:B:1869:GLN:HG3    | 2.21                     | 0.41              |
| 18:B8:745:ILE:O      | 18:B8:749:HIS:HB3    | 2.21                     | 0.41              |
| 18:B8:938:LEU:HD11   | 18:B8:1005:TYR:CE1   | 2.56                     | 0.41              |
| 18:B8:1661:TYR:CE1   | 18:B8:1689:TYR:HE2   | 2.39                     | 0.41              |
| 18:B8:1700:LEU:CD2   | 18:B8:1833:PHE:CE2   | 3.03                     | 0.41              |
| 19:4:184:SER:HB3     | 20:E:455:TYR:CD1     | 2.56                     | 0.41              |
| 19:4:220:TRP:CD2     | 19:4:227:LEU:HD13    | 2.56                     | 0.41              |
| 19:4:252:ARG:HD3     | 19:4:288:SER:OG      | 2.21                     | 0.41              |
| 20:E8:319:ARG:HB3    | 20:E8:320:PRO:CD     | 2.46                     | 0.41              |
| 20:E8:434:TRP:CD1    | 24:D40:72:GLU:HG2    | 2.56                     | 0.41              |
| 21:H:271:LEU:HD21    | 22:I:254:ILE:HG21    | 1.98                     | 0.41              |
| 22:I:204:PRO:HA      | 22:I:209:TRP:CZ3     | 2.56                     | 0.41              |
| 21:H8:280:LEU:CD1    | 22:I8:263:LEU:HD23   | 2.51                     | 0.41              |
| 21:H16:193:LEU:CD2   | 21:H16:195:GLN:HE21  | 2.18                     | 0.41              |
| 21:H16:280:LEU:CD1   | 22:I16:263:LEU:HD23  | 2.51                     | 0.41              |
| 24:D:622:ASP:HB2     | 24:D:649:ILE:HD11    | 2.03                     | 0.41              |
| 24:D32:1170:VAL:HG22 | 24:D32:1232:VAL:HG22 | 2.01                     | 0.41              |
| 24:D40:207:ASP:HA    | 24:D40:252:VAL:HG11  | 2.03                     | 0.41              |
| 24:D40:865:VAL:HG21  | 24:D40:928:THR:CG2   | 2.47                     | 0.41              |
| 10:C32:994:LEU:CD1   | 10:C32:1026:LEU:HD11 | 2.51                     | 0.41              |
| 1:R16:1124:TRP:HZ3   | 1:R16:1170:LEU:O     | 1.99                     | 0.41              |
| 5:P8:96:VAL:CG1      | 5:P8:481:ILE:CD1     | 2.98                     | 0.41              |
| 7:Q8:183:ARG:CZ      | 7:Q8:231:HIS:CE1     | 3.03                     | 0.41              |
| 5:P16:214:LEU:HD12   | 5:P16:245:TRP:HZ3    | 1.86                     | 0.41              |
| 5:P16:510:ILE:CD1    | 7:Q16:183:ARG:NH1    | 2.72                     | 0.41              |
| 5:P16:558:LEU:HB3    | 5:P16:594:ILE:HD13   | 2.03                     | 0.41              |
| 7:Q16:250:GLY:N      | 7:Q16:282:SER:O      | 2.54                     | 0.41              |
| 8:L16:1061:VAL:HG22  | 8:L16:1068:PHE:CD2   | 2.56                     | 0.41              |
| 9:K:601:VAL:CG1      | 9:K:604:SER:OG       | 2.54                     | 0.41              |
| 9:K:751:LEU:CD2      | 9:K:754:ARG:CD       | 2.97                     | 0.41              |
| 9:K:774:LEU:HD22     | 9:K:842:ILE:HD12     | 2.03                     | 0.41              |
| 10:C16:1449:GLU:OE1  | 24:D8:1151:SER:HB2   | 2.21                     | 0.41              |
| 10:C24:987:TYR:O     | 10:C24:988:GLN:C     | 2.62                     | 0.41              |
| 10:C24:1109:VAL:C    | 10:C24:1111:SER:N    | 2.79                     | 0.41              |
| 10:C24:1560:GLN:OE1  | 10:C24:1601:TYR:HD1  | 1.96                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C:267:LEU:CB     | 10:C:316:ILE:HD12   | 2.51                     | 0.41              |
| 10:C:267:LEU:CD1    | 10:C:316:ILE:HD12   | 2.50                     | 0.41              |
| 10:C8:803:ARG:HH21  | 10:C8:808:PRO:HG3   | 1.86                     | 0.41              |
| 11:A16:56:ALA:O     | 11:A16:58:SER:N     | 2.54                     | 0.41              |
| 17:F:74:ILE:HG22    | 17:F:76:ASP:H       | 1.86                     | 0.41              |
| 11:A32:787:ASP:HA   | 11:A32:788:PRO:HD3  | 1.86                     | 0.41              |
| 18:B:740:PHE:O      | 18:B:744:TYR:HB3    | 2.21                     | 0.41              |
| 18:B:749:HIS:O      | 18:B:754:TYR:OH     | 2.31                     | 0.41              |
| 18:B:980:LYS:O      | 18:B:981:GLN:C      | 2.63                     | 0.41              |
| 18:B:1398:LYS:CE    | 18:B:1450:ILE:HD11  | 2.51                     | 0.41              |
| 18:B:1590:LEU:HD13  | 18:B:1620:TRP:CZ3   | 2.56                     | 0.41              |
| 18:B8:467:ILE:HD11  | 18:B8:559:LEU:CD1   | 2.50                     | 0.41              |
| 18:B8:586:VAL:HB    | 18:B8:593:CYS:SG    | 2.61                     | 0.41              |
| 18:B8:1158:VAL:CG1  | 18:B8:1338:GLN:O    | 2.68                     | 0.41              |
| 19:48:253:GLY:HA3   | 19:48:273:ARG:NH2   | 2.36                     | 0.41              |
| 22:I:203:GLN:O      | 22:I:209:TRP:CE3    | 2.74                     | 0.41              |
| 22:I8:307:VAL:O     | 22:I8:311:VAL:HG23  | 2.20                     | 0.41              |
| 21:H24:262:GLU:OE1  | 22:I24:259:THR:OG1  | 2.36                     | 0.41              |
| 24:D16:1296:SER:O   | 24:D16:1343:LYS:HE3 | 2.21                     | 0.41              |
| 24:D24:622:ASP:HB2  | 24:D24:649:ILE:HD11 | 2.03                     | 0.41              |
| 24:D24:1284:ILE:CD1 | 24:D24:1319:ALA:HA  | 2.51                     | 0.41              |
| 24:D32:1099:ARG:O   | 24:D32:1099:ARG:CG  | 2.61                     | 0.41              |
| 10:C32:97:LEU:HD21  | 10:C32:123:TRP:HB2  | 2.03                     | 0.41              |
| 10:C32:452:LEU:HG   | 10:C32:453:LEU:HG   | 2.02                     | 0.41              |
| 10:C32:553:LEU:HD23 | 10:C32:595:THR:CG2  | 2.44                     | 0.41              |
| 10:C32:821:ILE:HD12 | 10:C32:861:ILE:HG21 | 2.01                     | 0.41              |
| 1:R:1248:PRO:C      | 1:R:1250:ASP:H      | 2.28                     | 0.41              |
| 1:R:1424:LYS:NZ     | 6:O:108:SER:OG      | 2.45                     | 0.41              |
| 2:M:180:ALA:O       | 2:M:184:GLY:HA3     | 2.21                     | 0.41              |
| 2:M:456:ARG:NH2     | 8:L:303:ARG:HH11    | 2.19                     | 0.41              |
| 2:M:810:LEU:CD2     | 2:M:819:GLN:HA      | 2.51                     | 0.41              |
| 1:R8:1248:PRO:C     | 1:R8:1250:ASP:H     | 2.28                     | 0.41              |
| 2:M8:565:THR:HG21   | 2:M8:570:ASP:OD2    | 2.21                     | 0.41              |
| 2:M8:763:ASP:OD1    | 2:M8:818:THR:CG2    | 2.68                     | 0.41              |
| 1:R16:672:LYS:HZ2   | 1:R16:842:ASP:CG    | 2.28                     | 0.41              |
| 1:R16:1078:SER:CB   | 5:P16:713:LEU:CD2   | 2.58                     | 0.41              |
| 2:M16:187:PHE:HA    | 3:N16:15:HIS:O      | 2.21                     | 0.41              |
| 2:M16:336:SER:O     | 2:M16:337:ASP:C     | 2.61                     | 0.41              |
| 5:P:143:ASN:C       | 5:P:145:ILE:N       | 2.78                     | 0.41              |
| 5:P:538:LYS:HB3     | 6:O:88:LEU:HD23     | 2.03                     | 0.41              |
| 5:P:539:HIS:CG      | 6:O:95:LEU:HD21     | 2.56                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:P:569:VAL:C       | 5:P:643:PHE:CE2     | 2.94                     | 0.41              |
| 5:P:663:LEU:HD23    | 5:P:667:GLN:HB3     | 2.03                     | 0.41              |
| 6:O:179:LYS:CE      | 6:O:183:GLN:OE1     | 2.56                     | 0.41              |
| 7:Q:236:HIS:ND1     | 7:Q:237:PRO:HD2     | 2.36                     | 0.41              |
| 5:P8:558:LEU:HB3    | 5:P8:594:ILE:HD13   | 2.03                     | 0.41              |
| 7:Q8:88:ASN:C       | 7:Q8:89:GLY:O       | 2.64                     | 0.41              |
| 7:Q8:259:TRP:CD1    | 7:Q8:259:TRP:N      | 2.89                     | 0.41              |
| 5:P16:16:PHE:CD1    | 6:O16:311:LEU:CG    | 3.04                     | 0.41              |
| 5:P16:71:VAL:HG11   | 6:O16:17:TRP:HZ2    | 1.86                     | 0.41              |
| 5:P16:188:LEU:CD2   | 5:P16:380:MET:CE    | 2.96                     | 0.41              |
| 5:P16:207:HIS:CB    | 5:P16:208:PRO:HD2   | 2.46                     | 0.41              |
| 5:P16:465:TYR:CE1   | 5:P16:482:TYR:CZ    | 3.07                     | 0.41              |
| 5:P16:499:TYR:HD2   | 6:O16:178:MET:SD    | 2.35                     | 0.41              |
| 6:O16:54:VAL:CG1    | 6:O16:85:TRP:NE1    | 2.68                     | 0.41              |
| 6:O16:54:VAL:HA     | 6:O16:85:TRP:CZ2    | 2.56                     | 0.41              |
| 6:O16:90:GLU:CD     | 6:O16:98:LYS:HZ3    | 2.29                     | 0.41              |
| 7:Q16:231:HIS:NE2   | 7:Q16:283:GLU:OE2   | 2.40                     | 0.41              |
| 8:L8:1069:LEU:HD11  | 9:K8:1086:VAL:CG1   | 2.36                     | 0.41              |
| 8:L16:1062:ALA:HB2  | 9:K16:1083:ILE:HD11 | 2.02                     | 0.41              |
| 9:K:688:GLN:O       | 9:K:692:GLU:HG3     | 2.21                     | 0.41              |
| 9:K8:585:GLU:HA     | 9:K8:622:VAL:HG11   | 2.02                     | 0.41              |
| 9:K8:774:LEU:HD22   | 9:K8:842:ILE:HD12   | 2.03                     | 0.41              |
| 9:K8:872:THR:HG23   | 9:K8:907:ILE:HG21   | 2.03                     | 0.41              |
| 9:K8:1074:ARG:CD    | 9:K8:1107:LEU:HD11  | 2.51                     | 0.41              |
| 9:K8:1110:GLN:HA    | 9:K8:1132:LEU:HD21  | 2.02                     | 0.41              |
| 9:K8:1277:ALA:O     | 9:K8:1278:GLU:C     | 2.56                     | 0.41              |
| 10:C16:8:VAL:HG21   | 10:C16:129:ASP:O    | 2.21                     | 0.41              |
| 10:C16:452:LEU:HD23 | 10:C16:452:LEU:N    | 2.20                     | 0.41              |
| 10:C16:615:GLU:CA   | 10:C16:619:LEU:HD12 | 2.49                     | 0.41              |
| 10:C16:664:ASN:O    | 10:C16:668:ALA:N    | 2.42                     | 0.41              |
| 10:C16:994:LEU:HD11 | 10:C16:1026:LEU:CD1 | 2.50                     | 0.41              |
| 10:C16:1009:GLN:HB3 | 10:C16:1192:ARG:NH1 | 2.36                     | 0.41              |
| 10:C16:1109:VAL:C   | 10:C16:1111:SER:N   | 2.79                     | 0.41              |
| 10:C16:1314:GLU:OE1 | 10:C16:1396:SER:OG  | 2.38                     | 0.41              |
| 10:C16:1708:ARG:HB2 | 10:C16:1730:ILE:CD1 | 2.50                     | 0.41              |
| 10:C16:1814:LYS:NZ  | 23:J32:738:MET:CG   | 2.83                     | 0.41              |
| 11:A24:11:THR:HG21  | 22:I8:162:GLN:CD    | 2.41                     | 0.41              |
| 11:A24:56:ALA:O     | 11:A24:58:SER:N     | 2.54                     | 0.41              |
| 11:A24:445:ASN:CB   | 17:F:65:ARG:CZ      | 2.63                     | 0.41              |
| 11:A24:650:GLY:HA2  | 11:A24:659:ARG:NH2  | 2.36                     | 0.41              |
| 11:A24:696:ILE:HD13 | 11:A24:725:GLY:N    | 2.36                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:C24:62:ILE:CD1   | 10:C24:95:VAL:HG21  | 2.51                     | 0.41              |
| 10:C24:228:ARG:CZ   | 10:C24:277:SER:CB   | 2.94                     | 0.41              |
| 10:C24:555:LYS:HD3  | 10:C24:555:LYS:HA   | 1.77                     | 0.41              |
| 10:C24:897:MET:HE1  | 10:C24:961:GLY:HA2  | 2.02                     | 0.41              |
| 10:C24:1071:GLN:O   | 10:C24:1072:ASP:C   | 2.54                     | 0.41              |
| 10:C24:1278:ASP:OD1 | 21:H24:282:GLU:CG   | 2.68                     | 0.41              |
| 11:A40:353:LEU:HD11 | 11:A40:381:TRP:HZ3  | 1.85                     | 0.41              |
| 11:A40:519:MET:HE2  | 11:A40:519:MET:HA   | 2.03                     | 0.41              |
| 11:A40:631:GLU:O    | 11:A40:632:ARG:HB2  | 2.20                     | 0.41              |
| 11:A40:650:GLY:HA2  | 11:A40:659:ARG:NH2  | 2.36                     | 0.41              |
| 12:A:519:MET:HE2    | 12:A:519:MET:HA     | 2.03                     | 0.41              |
| 13:V:758:CYS:O      | 13:V:762:LEU:HB2    | 2.21                     | 0.41              |
| 13:V:836:LEU:HD23   | 14:W:716:PHE:HE1    | 1.85                     | 0.41              |
| 14:W:514:THR:HA     | 14:W:607:ARG:NH1    | 2.36                     | 0.41              |
| 14:W:598:ILE:CG1    | 14:W:626:LEU:CD2    | 2.92                     | 0.41              |
| 10:C:271:PHE:HZ     | 10:C:296:PHE:CZ     | 2.38                     | 0.41              |
| 10:C:803:ARG:HH21   | 10:C:808:PRO:HG3    | 1.86                     | 0.41              |
| 10:C:994:LEU:CD1    | 10:C:1026:LEU:HD11  | 2.51                     | 0.41              |
| 10:C8:31:HIS:CE1    | 10:C8:35:ASN:HD21   | 2.38                     | 0.41              |
| 10:C8:267:LEU:CD1   | 10:C8:316:ILE:HD12  | 2.51                     | 0.41              |
| 10:C8:275:ALA:HB1   | 10:C8:326:LEU:HD13  | 2.03                     | 0.41              |
| 10:C8:643:LEU:CG    | 10:C8:656:THR:OG1   | 2.69                     | 0.41              |
| 10:C8:761:VAL:HG21  | 10:C8:826:TYR:CA    | 2.43                     | 0.41              |
| 10:C8:994:LEU:CD1   | 10:C8:1026:LEU:HD11 | 2.51                     | 0.41              |
| 10:C8:1043:ALA:O    | 10:C8:1047:ILE:HG13 | 2.21                     | 0.41              |
| 10:C8:1314:GLU:OE1  | 10:C8:1318:ARG:NH2  | 2.38                     | 0.41              |
| 10:C8:1764:ASN:OD1  | 10:C8:1825:LEU:HD11 | 2.20                     | 0.41              |
| 11:A16:11:THR:HG21  | 22:I:162:GLN:HG3    | 2.03                     | 0.41              |
| 11:A16:650:GLY:HA2  | 11:A16:659:ARG:NH2  | 2.36                     | 0.41              |
| 17:F8:74:ILE:HG22   | 17:F8:76:ASP:H      | 1.86                     | 0.41              |
| 11:A32:159:LYS:HZ1  | 18:B8:1918:ARG:HE   | 1.67                     | 0.41              |
| 11:A32:357:TYR:HB3  | 11:A32:360:GLU:OE2  | 2.21                     | 0.41              |
| 11:A32:696:ILE:HD13 | 11:A32:725:GLY:N    | 2.36                     | 0.41              |
| 11:A32:845:THR:HB   | 24:D32:1297:HIS:CE1 | 2.55                     | 0.41              |
| 18:B:208:LEU:HD13   | 18:B:260:ALA:O      | 2.21                     | 0.41              |
| 18:B:374:ILE:CG2    | 18:B:380:LEU:CD1    | 2.99                     | 0.41              |
| 18:B:1158:VAL:CG1   | 18:B:1338:GLN:O     | 2.68                     | 0.41              |
| 18:B:1553:SER:OG    | 18:B:1556:SER:HB3   | 2.20                     | 0.41              |
| 18:B:1700:LEU:HD23  | 18:B:1833:PHE:CG    | 2.56                     | 0.41              |
| 18:B8:86:LYS:HE2    | 18:B8:123:LEU:CG    | 2.50                     | 0.41              |
| 18:B8:347:SER:OG    | 18:B8:350:LEU:HD12  | 2.21                     | 0.41              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 18:B8:740:PHE:O      | 18:B8:744:TYR:HB3   | 2.21                     | 0.41              |
| 18:B8:1072:LEU:HD22  | 18:B8:1076:GLU:HB3  | 2.03                     | 0.41              |
| 18:B8:1098:MET:CE    | 18:B8:1142:PHE:CB   | 2.99                     | 0.41              |
| 18:B8:1398:LYS:CE    | 18:B8:1450:ILE:HD11 | 2.51                     | 0.41              |
| 18:B8:1418:ALA:HB3   | 18:B8:1422:LEU:HD12 | 2.02                     | 0.41              |
| 18:B8:1676:VAL:O     | 18:B8:1676:VAL:HG12 | 2.21                     | 0.41              |
| 19:4:94:VAL:O        | 19:4:95:THR:C       | 2.63                     | 0.41              |
| 20:E:38:PHE:CE2      | 20:E:122:PHE:CE1    | 3.09                     | 0.41              |
| 19:48:31:GLN:OE1     | 19:48:41:VAL:HG23   | 2.20                     | 0.41              |
| 19:48:282:GLU:O      | 19:48:286:TRP:HA    | 2.20                     | 0.41              |
| 20:E8:208:VAL:HG12   | 20:E8:212:LYS:HB3   | 2.03                     | 0.41              |
| 21:H:294:PRO:HA      | 21:H:300:ARG:NH2    | 2.36                     | 0.41              |
| 21:H8:141:THR:O      | 21:H8:143:PRO:HD3   | 2.20                     | 0.41              |
| 21:H8:261:ILE:HD12   | 22:I8:195:ALA:HB1   | 2.02                     | 0.41              |
| 22:I8:304:LEU:HB3    | 22:I8:305:PRO:CD    | 2.43                     | 0.41              |
| 21:H24:280:LEU:CD1   | 22:I24:263:LEU:HD23 | 2.51                     | 0.41              |
| 10:C32:267:LEU:CB    | 10:C32:316:ILE:HD12 | 2.51                     | 0.41              |
| 10:C32:585:PRO:HA    | 10:C32:586:PRO:HD3  | 1.90                     | 0.41              |
| 10:C32:792:PHE:O     | 10:C32:850:ARG:NH2  | 2.53                     | 0.41              |
| 10:C32:1009:GLN:HB3  | 10:C32:1192:ARG:NH1 | 2.36                     | 0.41              |
| 10:C32:1465:LEU:HD11 | 12:A48:128:PHE:CD2  | 2.56                     | 0.41              |
| 10:C32:1624:LEU:HD22 | 10:C32:1632:LEU:CD1 | 2.50                     | 0.41              |
| 12:A48:401:GLU:HG3   | 12:A48:405:ARG:HE   | 1.85                     | 0.41              |
| 12:A48:542:VAL:HG21  | 12:A48:596:THR:HG23 | 2.03                     | 0.41              |
| 12:A48:548:SER:CB    | 12:A48:559:VAL:HG13 | 2.51                     | 0.41              |
| 12:A48:567:SER:OG    | 12:A48:619:MET:HE1  | 2.21                     | 0.41              |
| 12:A48:631:GLU:O     | 12:A48:632:ARG:HB2  | 2.20                     | 0.41              |
| 1:R:1424:LYS:HZ1     | 6:O:134:ARG:HH22    | 1.62                     | 0.41              |
| 1:R:1473:HIS:HD2     | 6:O:160:LEU:HD13    | 1.84                     | 0.41              |
| 2:M:517:PRO:HB2      | 2:M:519:TYR:CE1     | 2.56                     | 0.41              |
| 1:R8:1431:ARG:O      | 2:M8:177:VAL:HG11   | 2.19                     | 0.41              |
| 2:M8:174:ARG:O       | 3:N8:212:TRP:HH2    | 2.03                     | 0.41              |
| 2:M8:385:LEU:CD1     | 2:M8:396:PHE:HD2    | 2.33                     | 0.41              |
| 1:R16:1393:PRO:HG3   | 1:R16:1416:TYR:OH   | 2.21                     | 0.41              |
| 1:R16:1470:GLN:NE2   | 6:O16:162:THR:N     | 2.41                     | 0.41              |
| 2:M16:370:LEU:O      | 2:M16:374:VAL:HG22  | 2.22                     | 0.41              |
| 2:M16:377:ARG:NH2    | 2:M16:477:ASP:HB3   | 2.36                     | 0.41              |
| 5:P8:402:LEU:CD1     | 5:P8:433:LEU:HB3    | 2.51                     | 0.41              |
| 5:P8:539:HIS:CG      | 6:O8:95:LEU:HD21    | 2.56                     | 0.41              |
| 7:Q8:250:GLY:N       | 7:Q8:282:SER:O      | 2.54                     | 0.41              |
| 7:Q8:254:ALA:HB3     | 7:Q8:302:ILE:CD1    | 2.50                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5:P16:510:ILE:HD13   | 7:Q16:183:ARG:HH12   | 1.81                     | 0.41              |
| 6:O16:179:LYS:CD     | 6:O16:183:GLN:CD     | 2.55                     | 0.41              |
| 9:K:897:LEU:CD2      | 9:K:901:TRP:CZ2      | 3.04                     | 0.41              |
| 9:K:1236:ASN:HA      | 9:K:1237:PRO:HD3     | 1.94                     | 0.41              |
| 9:K8:1048:GLN:HE22   | 9:K8:1128:ARG:CA     | 2.33                     | 0.41              |
| 10:C16:585:PRO:HA    | 10:C16:586:PRO:HD3   | 1.90                     | 0.41              |
| 10:C16:663:ILE:HG22  | 10:C16:667:ILE:CG1   | 2.51                     | 0.41              |
| 10:C16:988:GLN:HE21  | 10:C16:1064:PHE:HE1  | 1.59                     | 0.41              |
| 10:C16:1309:ARG:NE   | 10:C16:1311:GLU:O    | 2.53                     | 0.41              |
| 10:C16:1599:ASP:OD2  | 10:C16:1604:VAL:CB   | 2.66                     | 0.41              |
| 10:C16:1757:GLN:HG2  | 11:A24:140:TRP:CE2   | 2.56                     | 0.41              |
| 11:A24:519:MET:HE2   | 11:A24:519:MET:HA    | 2.03                     | 0.41              |
| 10:C24:234:VAL:HG21  | 10:C24:286:ILE:CD1   | 2.50                     | 0.41              |
| 10:C24:399:HIS:HA    | 10:C24:400:PRO:HD3   | 1.89                     | 0.41              |
| 10:C24:615:GLU:C     | 10:C24:619:LEU:HD12  | 2.46                     | 0.41              |
| 10:C24:1009:GLN:HB3  | 10:C24:1192:ARG:NH1  | 2.36                     | 0.41              |
| 10:C24:1271:PHE:CZ   | 10:C24:1284:ASP:HB3  | 2.37                     | 0.41              |
| 10:C24:1348:LEU:HD13 | 10:C24:1359:ILE:HG13 | 2.02                     | 0.41              |
| 11:A40:567:SER:OG    | 11:A40:619:MET:HE1   | 2.20                     | 0.41              |
| 11:A40:696:ILE:HD11  | 11:A40:728:ILE:HD12  | 1.92                     | 0.41              |
| 12:A:426:ILE:O       | 12:A:459:ARG:NH2     | 2.54                     | 0.41              |
| 14:W:552:GLU:O       | 14:W:553:MET:HE2     | 2.20                     | 0.41              |
| 14:W:716:PHE:CE1     | 14:W:720:LEU:HD11    | 2.56                     | 0.41              |
| 10:C:1285:VAL:CB     | 10:C:1738:MET:CE     | 2.85                     | 0.41              |
| 10:C8:453:LEU:CD2    | 10:C8:459:LEU:HD22   | 2.35                     | 0.41              |
| 10:C8:847:ARG:CD     | 10:C8:903:ASN:CG     | 2.94                     | 0.41              |
| 10:C8:1129:VAL:CG1   | 10:C8:1130:SER:N     | 2.81                     | 0.41              |
| 11:A16:348:GLN:HB3   | 11:A16:364:ILE:HD13  | 2.02                     | 0.41              |
| 11:A16:357:TYR:HB3   | 11:A16:360:GLU:OE2   | 2.21                     | 0.41              |
| 11:A16:426:ILE:O     | 11:A16:459:ARG:NH2   | 2.54                     | 0.41              |
| 11:A16:542:VAL:HG21  | 11:A16:596:THR:HG23  | 2.03                     | 0.41              |
| 11:A32:233:ALA:O     | 11:A32:236:THR:OG1   | 2.33                     | 0.41              |
| 11:A32:326:TYR:HE1   | 17:F24:77:TYR:CB     | 2.10                     | 0.41              |
| 11:A32:415:TYR:CE2   | 11:A32:420:LEU:HD22  | 2.56                     | 0.41              |
| 18:B:28:LEU:HD23     | 18:B:152:HIS:CE1     | 2.56                     | 0.41              |
| 18:B:52:SER:CB       | 18:B:178:ARG:NH2     | 2.84                     | 0.41              |
| 18:B8:52:SER:CB      | 18:B8:178:ARG:NH2    | 2.84                     | 0.41              |
| 18:B8:208:LEU:HD13   | 18:B8:260:ALA:O      | 2.21                     | 0.41              |
| 18:B8:374:ILE:CG2    | 18:B8:380:LEU:CD1    | 2.99                     | 0.41              |
| 19:4:97:LEU:HD21     | 19:4:232:TYR:CD2     | 2.56                     | 0.41              |
| 19:4:125:ILE:HD11    | 19:4:139:LEU:HD11    | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 19:48:103:GLN:HE22  | 19:48:411:LEU:HD13  | 1.82                     | 0.41              |
| 19:48:189:LEU:CD2   | 19:48:203:LEU:HD21  | 2.46                     | 0.41              |
| 20:E8:24:ILE:N      | 20:E8:25:PRO:HD2    | 2.36                     | 0.41              |
| 21:H16:141:THR:O    | 21:H16:143:PRO:HD3  | 2.20                     | 0.41              |
| 24:D16:1284:ILE:CD1 | 24:D16:1319:ALA:HA  | 2.51                     | 0.41              |
| 24:D32:1284:ILE:CD1 | 24:D32:1319:ALA:HA  | 2.51                     | 0.41              |
| 24:D40:1109:LEU:HB2 | 24:D40:1127:ARG:HD3 | 2.03                     | 0.41              |
| 10:C32:320:TRP:NE1  | 10:C32:324:LEU:HD11 | 2.35                     | 0.41              |
| 10:C32:1593:TRP:CE2 | 10:C32:1603:PHE:HD2 | 2.37                     | 0.41              |
| 10:C32:1757:GLN:HG2 | 12:A48:140:TRP:CE2  | 2.56                     | 0.41              |
| 2:M:342:VAL:CG1     | 2:M:343:MET:N       | 2.59                     | 0.40              |
| 1:R8:1269:LEU:CB    | 5:P8:684:ARG:HG2    | 2.39                     | 0.40              |
| 2:M8:377:ARG:NH2    | 2:M8:477:ASP:HB3    | 2.36                     | 0.40              |
| 2:M8:496:LEU:HB2    | 2:M8:497:PRO:HD3    | 2.03                     | 0.40              |
| 2:M8:760:GLU:HA     | 2:M8:761:PRO:HD3    | 1.89                     | 0.40              |
| 1:R16:1156:GLU:OE2  | 1:R16:1156:GLU:HA   | 2.21                     | 0.40              |
| 2:M16:399:THR:HA    | 2:M16:484:LEU:HD21  | 2.03                     | 0.40              |
| 3:N16:154:THR:OG1   | 3:N16:213:VAL:O     | 2.35                     | 0.40              |
| 5:P:106:ARG:NH1     | 5:P:458:GLU:OE1     | 2.52                     | 0.40              |
| 5:P:558:LEU:HB3     | 5:P:594:ILE:HD13    | 2.03                     | 0.40              |
| 7:Q:22:VAL:O        | 7:Q:23:ARG:NH1      | 2.50                     | 0.40              |
| 7:Q:102:ALA:HB1     | 7:Q:137:VAL:HB      | 2.02                     | 0.40              |
| 7:Q:183:ARG:CZ      | 7:Q:231:HIS:CE1     | 3.03                     | 0.40              |
| 7:Q:222:PHE:O       | 7:Q:223:GLN:C       | 2.62                     | 0.40              |
| 7:Q:251:THR:HA      | 7:Q:267:SER:O       | 2.21                     | 0.40              |
| 7:Q:331:CYS:HB3     | 7:Q:352:TRP:CD2     | 2.56                     | 0.40              |
| 5:P8:10:GLY:HA2     | 5:P8:26:TYR:HE1     | 1.83                     | 0.40              |
| 5:P8:32:LEU:HD13    | 5:P8:55:ARG:HD2     | 2.03                     | 0.40              |
| 5:P8:214:LEU:HD21   | 5:P8:236:VAL:HG12   | 2.01                     | 0.40              |
| 5:P8:510:ILE:HD13   | 7:Q8:183:ARG:HH12   | 1.81                     | 0.40              |
| 5:P8:538:LYS:HB3    | 6:O8:88:LEU:HD23    | 2.03                     | 0.40              |
| 6:O8:190:ALA:CB     | 6:O8:232:LEU:HD11   | 2.52                     | 0.40              |
| 7:Q8:125:TYR:CB     | 7:Q8:168:LEU:HG     | 2.47                     | 0.40              |
| 7:Q8:314:LEU:CD2    | 7:Q8:327:LEU:HD12   | 2.51                     | 0.40              |
| 9:K:1137:LEU:HD23   | 9:K:1173:ASN:ND2    | 2.23                     | 0.40              |
| 9:K8:697:LEU:HA     | 9:K8:764:VAL:HG11   | 2.02                     | 0.40              |
| 9:K16:637:HIS:CE1   | 9:K16:754:ARG:HD3   | 2.55                     | 0.40              |
| 9:K16:1249:MET:HG2  | 9:K16:1254:PHE:CE1  | 2.56                     | 0.40              |
| 10:C16:168:ARG:HH12 | 10:C16:229:PRO:CA   | 2.31                     | 0.40              |
| 10:C16:267:LEU:CB   | 10:C16:316:ILE:HD12 | 2.51                     | 0.40              |
| 10:C16:424:ASP:HA   | 10:C16:425:PRO:HD3  | 1.81                     | 0.40              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 10:C16:535:MET:HA    | 10:C16:536:PRO:HD3   | 1.89                     | 0.40              |
| 10:C16:792:PHE:O     | 10:C16:850:ARG:NH2   | 2.53                     | 0.40              |
| 10:C16:1014:SER:O    | 10:C16:1018:GLN:HG3  | 2.20                     | 0.40              |
| 10:C16:1283:LEU:CD1  | 10:C16:1357:LEU:HD13 | 2.49                     | 0.40              |
| 10:C16:1304:VAL:CG1  | 10:C16:1384:ILE:HD11 | 2.45                     | 0.40              |
| 10:C16:1314:GLU:OE1  | 10:C16:1318:ARG:NH2  | 2.38                     | 0.40              |
| 10:C24:8:VAL:HG21    | 10:C24:129:ASP:O     | 2.21                     | 0.40              |
| 10:C24:394:SER:HG    | 10:C24:452:LEU:HD11  | 1.79                     | 0.40              |
| 10:C24:696:GLN:OE1   | 10:C24:783:LEU:HD11  | 2.21                     | 0.40              |
| 10:C24:803:ARG:HH21  | 10:C24:808:PRO:HG3   | 1.85                     | 0.40              |
| 10:C24:821:ILE:HD11  | 10:C24:861:ILE:HD13  | 2.03                     | 0.40              |
| 10:C24:1335:ILE:HD11 | 10:C24:1362:ILE:HG22 | 2.03                     | 0.40              |
| 12:A:153:ARG:CD      | 10:C8:74:ASP:OD1     | 2.65                     | 0.40              |
| 12:A:381:TRP:NE1     | 12:A:386:GLY:HA2     | 2.36                     | 0.40              |
| 10:C:281:ASP:CG      | 24:D:1398:ARG:NE     | 2.79                     | 0.40              |
| 10:C:1009:GLN:HB3    | 10:C:1192:ARG:NH1    | 2.36                     | 0.40              |
| 10:C8:182:ASP:OD1    | 10:C8:182:ASP:N      | 2.52                     | 0.40              |
| 10:C8:267:LEU:CB     | 10:C8:316:ILE:HD12   | 2.51                     | 0.40              |
| 10:C8:707:ILE:HD11   | 10:C8:740:LEU:HD11   | 2.02                     | 0.40              |
| 10:C8:1109:VAL:C     | 10:C8:1111:SER:N     | 2.79                     | 0.40              |
| 10:C8:1127:THR:O     | 10:C8:1128:SER:C     | 2.62                     | 0.40              |
| 10:C8:1385:LEU:HD11  | 10:C8:1419:PHE:CD1   | 2.56                     | 0.40              |
| 10:C8:1503:VAL:HG21  | 10:C8:1515:VAL:HG21  | 2.02                     | 0.40              |
| 11:A16:415:TYR:CE2   | 11:A16:420:LEU:HD22  | 2.57                     | 0.40              |
| 11:A16:500:ASP:CG    | 11:A16:503:VAL:HG23  | 2.46                     | 0.40              |
| 11:A32:348:GLN:HB3   | 11:A32:364:ILE:HD13  | 2.02                     | 0.40              |
| 11:A32:542:VAL:HG21  | 11:A32:596:THR:HG23  | 2.03                     | 0.40              |
| 18:B:1072:LEU:HD22   | 18:B:1076:GLU:HB3    | 2.03                     | 0.40              |
| 18:B:1101:TYR:CZ     | 18:B:1105:LEU:HD11   | 2.54                     | 0.40              |
| 18:B8:864:LEU:HB3    | 18:B8:910:TYR:CZ     | 2.56                     | 0.40              |
| 18:B8:1518:VAL:O     | 18:B8:1522:LEU:HG    | 2.21                     | 0.40              |
| 18:B8:1527:THR:C     | 18:B8:1531:TRP:CD1   | 2.99                     | 0.40              |
| 18:B8:1666:PRO:HG2   | 18:B8:1731:PHE:CZ    | 2.56                     | 0.40              |
| 18:B8:1719:SER:N     | 18:B8:1720:PRO:CD    | 2.84                     | 0.40              |
| 19:4:14:GLU:HB3      | 19:4:439:LEU:HA      | 2.03                     | 0.40              |
| 19:4:282:GLU:O       | 19:4:286:TRP:HA      | 2.20                     | 0.40              |
| 20:E:175:LEU:HB2     | 20:E:176:PRO:HD3     | 2.02                     | 0.40              |
| 20:E:340:GLY:CA      | 20:E:341:TYR:N       | 2.71                     | 0.40              |
| 20:E:418:THR:C       | 20:E:420:LEU:N       | 2.73                     | 0.40              |
| 19:48:214:GLN:HG2    | 19:48:232:TYR:HE1    | 1.86                     | 0.40              |
| 19:48:392:ILE:HG22   | 19:48:393:VAL:N      | 2.36                     | 0.40              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:J32:644:ARG:HA    | 23:J32:647:MET:HE2   | 2.03                     | 0.40              |
| 22:I16:142:ARG:O     | 23:J16:571:TRP:NE1   | 2.54                     | 0.40              |
| 24:D8:207:ASP:HA     | 24:D8:252:VAL:HG11   | 2.03                     | 0.40              |
| 24:D8:1284:ILE:CD1   | 24:D8:1319:ALA:HA    | 2.51                     | 0.40              |
| 10:C32:228:ARG:CZ    | 10:C32:277:SER:CB    | 2.94                     | 0.40              |
| 10:C32:445:MET:HE1   | 10:C32:462:PHE:HZ    | 1.84                     | 0.40              |
| 10:C32:456:ASN:C     | 10:C32:458:VAL:N     | 2.76                     | 0.40              |
| 10:C32:817:HIS:HB3   | 10:C32:857:MET:SD    | 2.60                     | 0.40              |
| 10:C32:1043:ALA:O    | 10:C32:1047:ILE:HG13 | 2.21                     | 0.40              |
| 12:A48:357:TYR:HB3   | 12:A48:360:GLU:OE2   | 2.21                     | 0.40              |
| 1:R:768:LEU:HD22     | 1:R:768:LEU:N        | 2.36                     | 0.40              |
| 1:R:1022:TYR:CZ      | 24:D:1441:PRO:CB     | 3.01                     | 0.40              |
| 1:R:1393:PRO:HG3     | 1:R:1416:TYR:OH      | 2.21                     | 0.40              |
| 2:M:399:THR:HA       | 2:M:484:LEU:HD21     | 2.03                     | 0.40              |
| 3:N:5:LYS:HD2        | 10:C:518:ARG:HD2     | 2.04                     | 0.40              |
| 1:R8:1156:GLU:OE2    | 1:R8:1156:GLU:HA     | 2.22                     | 0.40              |
| 2:M8:370:LEU:O       | 2:M8:374:VAL:HG22    | 2.21                     | 0.40              |
| 2:M8:544:LEU:HG      | 2:M8:586:ALA:HB1     | 2.03                     | 0.40              |
| 2:M16:180:ALA:O      | 2:M16:184:GLY:HA3    | 2.21                     | 0.40              |
| 4:T:672:GLN:NE2      | 5:P:702:LEU:HD21     | 2.36                     | 0.40              |
| 5:P:71:VAL:HG11      | 6:O:17:TRP:HZ2       | 1.86                     | 0.40              |
| 5:P:565:LEU:O        | 5:P:568:SER:OG       | 2.36                     | 0.40              |
| 7:Q:149:VAL:CG2      | 7:Q:187:TRP:CE2      | 2.99                     | 0.40              |
| 7:Q:250:GLY:N        | 7:Q:282:SER:O        | 2.54                     | 0.40              |
| 5:P16:288:ARG:HB2    | 5:P16:289:PRO:HD2    | 2.01                     | 0.40              |
| 5:P16:538:LYS:HB3    | 6:O16:88:LEU:HD23    | 2.03                     | 0.40              |
| 7:Q16:183:ARG:CZ     | 7:Q16:231:HIS:CE1    | 3.03                     | 0.40              |
| 9:K:959:TRP:CD1      | 9:K:992:GLN:CD       | 2.99                     | 0.40              |
| 9:K:1022:ASP:OD1     | 9:K:1022:ASP:N       | 2.54                     | 0.40              |
| 9:K:1180:TRP:CE2     | 9:K:1261:MET:HG2     | 2.56                     | 0.40              |
| 9:K8:897:LEU:CD2     | 9:K8:901:TRP:CZ2     | 3.04                     | 0.40              |
| 10:C16:320:TRP:NE1   | 10:C16:324:LEU:HD11  | 2.36                     | 0.40              |
| 10:C16:470:HIS:HD2   | 10:C16:508:ILE:CD1   | 2.30                     | 0.40              |
| 10:C16:586:PRO:HD3   | 10:C16:650:ARG:NH1   | 2.30                     | 0.40              |
| 11:A24:41:GLU:HA     | 22:I8:307:VAL:HG22   | 2.04                     | 0.40              |
| 11:A24:504:TYR:HB3   | 11:A24:505:PRO:CD    | 2.45                     | 0.40              |
| 10:C24:1503:VAL:HG21 | 10:C24:1515:VAL:HG21 | 2.02                     | 0.40              |
| 12:A:788:PRO:HA      | 12:A:836:LYS:HE3     | 2.03                     | 0.40              |
| 14:W:645:HIS:CE1     | 15:J:572:ASP:CG      | 2.99                     | 0.40              |
| 14:W:711:ARG:CD      | 10:C8:1609:ASP:HB2   | 2.47                     | 0.40              |
| 10:C:47:PRO:HA       | 10:C:48:PRO:HD3      | 1.93                     | 0.40              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 10:C:62:ILE:CD1      | 10:C:95:VAL:HG21    | 2.51                     | 0.40              |
| 10:C8:1271:PHE:CD1   | 10:C8:1273:GLY:N    | 2.81                     | 0.40              |
| 10:C8:1541:PHE:O     | 10:C8:1542:PHE:C    | 2.60                     | 0.40              |
| 10:C8:1757:GLN:HG2   | 16:A8:140:TRP:CE2   | 2.56                     | 0.40              |
| 11:A16:259:ILE:HG23  | 11:A16:276:LEU:HD22 | 1.96                     | 0.40              |
| 11:A16:519:MET:HE2   | 11:A16:519:MET:HA   | 2.03                     | 0.40              |
| 11:A16:790:MET:O     | 11:A16:836:LYS:NZ   | 2.49                     | 0.40              |
| 11:A32:11:THR:HG21   | 22:I24:162:GLN:HG3  | 2.03                     | 0.40              |
| 11:A32:232:ASP:O     | 11:A32:236:THR:HG23 | 2.20                     | 0.40              |
| 11:A32:259:ILE:HG23  | 11:A32:276:LEU:CD2  | 2.51                     | 0.40              |
| 11:A32:426:ILE:O     | 11:A32:459:ARG:NH2  | 2.54                     | 0.40              |
| 11:A32:704:ILE:HG12  | 11:A32:760:LEU:CD1  | 2.49                     | 0.40              |
| 18:B:32:LEU:HD21     | 18:B:36:ILE:HG21    | 2.03                     | 0.40              |
| 18:B:251:PHE:HZ      | 18:B:267:VAL:HG11   | 1.86                     | 0.40              |
| 18:B:286:GLN:HB2     | 18:B:443:PHE:CE2    | 2.55                     | 0.40              |
| 18:B:714:VAL:HG13    | 18:B:715:ILE:N      | 2.37                     | 0.40              |
| 18:B:986:ALA:C       | 18:B:988:SER:N      | 2.78                     | 0.40              |
| 18:B:1848:VAL:HG11   | 18:B:1850:TYR:CE1   | 2.56                     | 0.40              |
| 18:B8:286:GLN:HB2    | 18:B8:443:PHE:CE2   | 2.55                     | 0.40              |
| 18:B8:313:ILE:HD12   | 18:B8:331:TRP:CG    | 2.45                     | 0.40              |
| 18:B8:692:LEU:HD12   | 18:B8:740:PHE:HB2   | 2.02                     | 0.40              |
| 20:E8:437:SER:C      | 20:E8:439:MET:N     | 2.52                     | 0.40              |
| 21:H:255:LEU:CD1     | 23:J32:655:GLU:CD   | 2.85                     | 0.40              |
| 22:I8:368:VAL:HG22   | 23:J8:591:LYS:HD2   | 2.03                     | 0.40              |
| 22:I24:142:ARG:O     | 23:J24:571:TRP:NE1  | 2.55                     | 0.40              |
| 24:D16:1376:VAL:HG11 | 24:D16:1430:TYR:CE2 | 2.56                     | 0.40              |
| 10:C32:8:VAL:HG21    | 10:C32:129:ASP:O    | 2.21                     | 0.40              |
| 10:C32:1163:LEU:C    | 10:C32:1166:SER:H   | 2.28                     | 0.40              |
| 10:C32:1385:LEU:HD23 | 10:C32:1389:ILE:CD1 | 2.47                     | 0.40              |
| 10:C32:1385:LEU:HD11 | 10:C32:1419:PHE:HD1 | 1.84                     | 0.40              |
| 10:C32:1405:TYR:CE2  | 12:A48:117:ILE:HG23 | 2.56                     | 0.40              |
| 12:A48:696:ILE:HD13  | 12:A48:725:GLY:N    | 2.36                     | 0.40              |
| 1:R:422:ARG:HH22     | 1:R:584:GLY:HA2     | 1.86                     | 0.40              |
| 1:R:1473:HIS:HD2     | 6:O:160:LEU:CB      | 2.34                     | 0.40              |
| 3:N:258:PHE:C        | 3:N:260:THR:H       | 2.29                     | 0.40              |
| 1:R8:1132:TYR:OH     | 1:R8:1214:ILE:HD13  | 2.19                     | 0.40              |
| 2:M8:162:ILE:CD1     | 2:M8:213:LEU:CD1    | 2.97                     | 0.40              |
| 1:R16:1269:LEU:HD13  | 5:P16:684:ARG:HG2   | 0.55                     | 0.40              |
| 2:M16:174:ARG:O      | 3:N16:212:TRP:HH2   | 2.03                     | 0.40              |
| 2:M16:496:LEU:HB2    | 2:M16:497:PRO:HD3   | 2.04                     | 0.40              |
| 2:M16:761:PRO:C      | 2:M16:763:ASP:H     | 2.30                     | 0.40              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 5:P:158:VAL:HG12     | 5:P:248:ILE:HG23    | 2.00                     | 0.40              |
| 5:P:346:ILE:O        | 5:P:346:ILE:HG22    | 2.21                     | 0.40              |
| 5:P:607:PHE:CE1      | 5:P:611:LEU:HD13    | 2.54                     | 0.40              |
| 6:O:54:VAL:HA        | 6:O:85:TRP:CZ2      | 2.56                     | 0.40              |
| 7:Q:259:TRP:CD1      | 7:Q:259:TRP:N       | 2.89                     | 0.40              |
| 5:P8:143:ASN:C       | 5:P8:145:ILE:N      | 2.78                     | 0.40              |
| 5:P8:614:VAL:C       | 5:P8:629:ARG:NH1    | 2.79                     | 0.40              |
| 7:Q8:251:THR:HA      | 7:Q8:267:SER:O      | 2.21                     | 0.40              |
| 5:P16:346:ILE:O      | 5:P16:346:ILE:HG22  | 2.21                     | 0.40              |
| 8:L8:614:GLU:OE2     | 8:L8:649:LYS:NZ     | 2.52                     | 0.40              |
| 8:L16:1071:LEU:CD2   | 9:K16:1284:MET:CE   | 2.87                     | 0.40              |
| 9:K8:683:GLN:HB3     | 9:K8:686:SER:OG     | 2.21                     | 0.40              |
| 9:K8:994:TYR:CE2     | 9:K8:1023:LEU:HD12  | 2.57                     | 0.40              |
| 9:K8:1050:GLU:C      | 9:K8:1052:SER:H     | 2.30                     | 0.40              |
| 10:C16:365:LEU:HD22  | 10:C16:370:ARG:CZ   | 2.52                     | 0.40              |
| 10:C16:803:ARG:HH21  | 10:C16:808:PRO:HG3  | 1.86                     | 0.40              |
| 10:C16:1126:ASP:OD1  | 24:D8:1069:GLY:CA   | 2.69                     | 0.40              |
| 11:A24:788:PRO:HA    | 11:A24:836:LYS:HE3  | 2.03                     | 0.40              |
| 11:A24:823:VAL:O     | 11:A24:830:ILE:HD13 | 2.20                     | 0.40              |
| 10:C24:535:MET:HA    | 10:C24:536:PRO:HD3  | 1.90                     | 0.40              |
| 10:C24:572:ILE:CG1   | 10:C24:606:MET:CE   | 2.90                     | 0.40              |
| 10:C24:1385:LEU:HD11 | 10:C24:1419:PHE:CD1 | 2.56                     | 0.40              |
| 10:C24:1405:TYR:CE2  | 11:A40:117:ILE:HG23 | 2.56                     | 0.40              |
| 10:C24:1449:GLU:OE2  | 24:D24:1151:SER:CA  | 2.69                     | 0.40              |
| 11:A40:41:GLU:HA     | 22:I16:307:VAL:HG22 | 2.04                     | 0.40              |
| 11:A40:357:TYR:HB3   | 11:A40:360:GLU:OE2  | 2.21                     | 0.40              |
| 12:A:374:PHE:CE2     | 12:A:426:ILE:HD11   | 2.54                     | 0.40              |
| 14:W:220:TYR:CE2     | 14:W:242:THR:HG21   | 2.55                     | 0.40              |
| 10:C:320:TRP:NE1     | 10:C:324:LEU:HD11   | 2.35                     | 0.40              |
| 10:C:821:ILE:HD12    | 10:C:861:ILE:HG21   | 2.01                     | 0.40              |
| 10:C:1314:GLU:OE1    | 10:C:1396:SER:OG    | 2.38                     | 0.40              |
| 10:C:1344:VAL:HG12   | 10:C:1348:LEU:HD12  | 2.02                     | 0.40              |
| 10:C8:365:LEU:HD22   | 10:C8:370:ARG:CZ    | 2.52                     | 0.40              |
| 10:C8:381:ILE:HG22   | 10:C8:385:TYR:CE2   | 2.57                     | 0.40              |
| 10:C8:456:ASN:C      | 10:C8:458:VAL:N     | 2.76                     | 0.40              |
| 10:C8:615:GLU:CA     | 10:C8:619:LEU:HD12  | 2.49                     | 0.40              |
| 10:C8:696:GLN:OE1    | 10:C8:783:LEU:HD11  | 2.21                     | 0.40              |
| 11:A16:798:PHE:HZ    | 11:A16:847:ARG:NH1  | 2.02                     | 0.40              |
| 11:A32:212:LYS:HG2   | 11:A32:588:GLU:HG3  | 2.03                     | 0.40              |
| 11:A32:548:SER:CB    | 11:A32:559:VAL:HG13 | 2.51                     | 0.40              |
| 11:A32:845:THR:HG21  | 24:D32:1297:HIS:CE1 | 2.56                     | 0.40              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 18:B:235:ARG:NH1     | 18:B:308:GLU:CB      | 2.82                     | 0.40              |
| 18:B8:472:SER:HA     | 18:B8:584:ARG:HH12   | 1.84                     | 0.40              |
| 18:B8:1590:LEU:HD13  | 18:B8:1620:TRP:CZ3   | 2.56                     | 0.40              |
| 20:E:339:LYS:C       | 20:E:340:GLY:O       | 2.63                     | 0.40              |
| 21:H:166:VAL:HG22    | 21:H:193:LEU:HD13    | 2.04                     | 0.40              |
| 22:I:142:ARG:O       | 23:J32:571:TRP:NE1   | 2.54                     | 0.40              |
| 24:D:1009:CYS:HB3    | 24:D:1013:HIS:CE1    | 2.55                     | 0.40              |
| 24:D16:1049:VAL:HB   | 24:D16:1050:PRO:HD3  | 2.04                     | 0.40              |
| 24:D24:94:ALA:HB1    | 24:D24:543:MET:HE1   | 2.00                     | 0.40              |
| 24:D32:622:ASP:HB2   | 24:D32:649:ILE:HD11  | 2.03                     | 0.40              |
| 24:D40:1296:SER:O    | 24:D40:1343:LYS:HE3  | 2.21                     | 0.40              |
| 24:D40:1376:VAL:HG11 | 24:D40:1430:TYR:CE2  | 2.56                     | 0.40              |
| 10:C32:1109:VAL:C    | 10:C32:1111:SER:N    | 2.79                     | 0.40              |
| 10:C32:1304:VAL:CG1  | 10:C32:1384:ILE:HD11 | 2.45                     | 0.40              |
| 10:C32:1756:LEU:HD11 | 10:C32:1815:VAL:CG1  | 2.51                     | 0.40              |
| 12:A48:426:ILE:O     | 12:A48:459:ARG:NH2   | 2.54                     | 0.40              |
| 1:R:1449:TRP:HE1     | 2:M:164:HIS:HB3      | 1.87                     | 0.40              |
| 2:M:250:LEU:CD1      | 2:M:286:SER:HB2      | 2.52                     | 0.40              |
| 2:M:420:CYS:CB       | 8:L:391:TRP:CH2      | 3.01                     | 0.40              |
| 1:R8:1393:PRO:HG3    | 1:R8:1416:TYR:OH     | 2.21                     | 0.40              |
| 1:R16:422:ARG:HH22   | 1:R16:584:GLY:HA2    | 1.86                     | 0.40              |
| 5:P:10:GLY:HA2       | 5:P:26:TYR:HE1       | 1.83                     | 0.40              |
| 5:P:96:VAL:CG1       | 5:P:481:ILE:CD1      | 2.98                     | 0.40              |
| 5:P:214:LEU:HD12     | 5:P:245:TRP:HZ3      | 1.86                     | 0.40              |
| 5:P8:16:PHE:CD1      | 6:O8:311:LEU:CG      | 3.04                     | 0.40              |
| 5:P8:71:VAL:HG11     | 6:O8:17:TRP:HZ2      | 1.86                     | 0.40              |
| 7:Q16:331:CYS:HB3    | 7:Q16:352:TRP:CD2    | 2.56                     | 0.40              |
| 9:K:585:GLU:CA       | 9:K:622:VAL:CG1      | 2.97                     | 0.40              |
| 9:K:930:THR:O        | 9:K:933:THR:OG1      | 2.39                     | 0.40              |
| 9:K8:1071:PHE:CE2    | 9:K8:1107:LEU:CD2    | 3.00                     | 0.40              |
| 9:K8:1180:TRP:CE2    | 9:K8:1261:MET:HG2    | 2.56                     | 0.40              |
| 10:C16:994:LEU:CD1   | 10:C16:1026:LEU:HD11 | 2.51                     | 0.40              |
| 10:C16:1465:LEU:HD11 | 11:A24:128:PHE:CD2   | 2.56                     | 0.40              |
| 10:C16:1503:VAL:HG21 | 10:C16:1515:VAL:HG21 | 2.02                     | 0.40              |
| 11:A24:259:ILE:HG23  | 11:A24:276:LEU:CD2   | 2.51                     | 0.40              |
| 10:C24:48:PRO:HA     | 10:C24:49:PRO:HD3    | 1.86                     | 0.40              |
| 10:C24:994:LEU:CD1   | 10:C24:1026:LEU:HD11 | 2.51                     | 0.40              |
| 10:C24:1449:GLU:CD   | 24:D24:1151:SER:CA   | 2.91                     | 0.40              |
| 10:C24:1756:LEU:HD11 | 10:C24:1815:VAL:CG1  | 2.52                     | 0.40              |
| 11:A40:157:LEU:HA    | 11:A40:158:PRO:HD3   | 1.97                     | 0.40              |
| 11:A40:381:TRP:NE1   | 11:A40:386:GLY:HA2   | 2.36                     | 0.40              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 11:A40:803:PRO:HB3   | 24:D24:1401:LEU:CG   | 2.34                     | 0.40              |
| 12:A:117:ILE:HG23    | 10:C:1405:TYR:CE2    | 2.56                     | 0.40              |
| 12:A:140:TRP:CE2     | 10:C:1757:GLN:HG2    | 2.56                     | 0.40              |
| 12:A:696:ILE:HD11    | 12:A:728:ILE:HD12    | 1.92                     | 0.40              |
| 10:C:586:PRO:HD3     | 10:C:650:ARG:NH1     | 2.30                     | 0.40              |
| 10:C:1335:ILE:HD11   | 10:C:1362:ILE:HG22   | 2.04                     | 0.40              |
| 10:C:1560:GLN:OE1    | 10:C:1601:TYR:HE1    | 2.00                     | 0.40              |
| 10:C8:1314:GLU:OE1   | 10:C8:1396:SER:OG    | 2.39                     | 0.40              |
| 11:A32:101:VAL:O     | 11:A32:105:LEU:HG    | 2.22                     | 0.40              |
| 11:A32:401:GLU:HG3   | 11:A32:405:ARG:HE    | 1.85                     | 0.40              |
| 18:B:12:TRP:NE1      | 18:B:75:HIS:CD2      | 2.90                     | 0.40              |
| 18:B:347:SER:OG      | 18:B:350:LEU:HD12    | 2.21                     | 0.40              |
| 18:B8:784:LEU:HG     | 18:B8:788:LEU:HD12   | 2.02                     | 0.40              |
| 18:B8:1793:ILE:O     | 18:B8:1793:ILE:HG22  | 2.20                     | 0.40              |
| 18:B8:1911:LEU:N     | 18:B8:1960:LEU:HD11  | 2.37                     | 0.40              |
| 19:4:67:SER:O        | 19:4:69:GLU:N        | 2.55                     | 0.40              |
| 19:4:171:TRP:CH2     | 19:4:192:SER:HB2     | 2.57                     | 0.40              |
| 20:E:6:VAL:HG12      | 20:E:7:PRO:HD2       | 2.04                     | 0.40              |
| 19:48:184:SER:HB3    | 20:E8:455:TYR:CD1    | 2.56                     | 0.40              |
| 21:H8:294:PRO:HA     | 21:H8:300:ARG:NH2    | 2.36                     | 0.40              |
| 21:H24:280:LEU:CD2   | 22:I24:262:LEU:HG    | 2.49                     | 0.40              |
| 24:D:313:VAL:HG21    | 24:D16:13:THR:CG2    | 2.51                     | 0.40              |
| 24:D8:1328:ASN:ND2   | 24:D16:729:LEU:CD2   | 2.84                     | 0.40              |
| 24:D24:207:ASP:HA    | 24:D24:252:VAL:HG11  | 2.03                     | 0.40              |
| 24:D24:1376:VAL:HG11 | 24:D24:1430:TYR:CE2  | 2.57                     | 0.40              |
| 24:D32:1376:VAL:HG11 | 24:D32:1430:TYR:CE2  | 2.57                     | 0.40              |
| 10:C32:33:ILE:HG21   | 10:C32:158:LEU:HD22  | 2.02                     | 0.40              |
| 10:C32:439:LEU:HA    | 10:C32:440:PRO:HD3   | 1.86                     | 0.40              |
| 10:C32:803:ARG:HH21  | 10:C32:808:PRO:HG3   | 1.86                     | 0.40              |
| 12:A48:519:MET:HE2   | 12:A48:519:MET:HA    | 2.03                     | 0.40              |
| 1:R:1132:TYR:CD2     | 1:R:1219:LEU:HD21    | 2.57                     | 0.40              |
| 2:M:385:LEU:CD1      | 2:M:396:PHE:HD2      | 2.33                     | 0.40              |
| 3:N:2:PRO:HB2        | 10:C:518:ARG:HH12    | 1.87                     | 0.40              |
| 1:R8:768:LEU:CD1     | 24:D40:1364:PRO:HD2  | 2.41                     | 0.40              |
| 1:R8:1059:ILE:CG2    | 24:D40:1435:ARG:HH12 | 2.30                     | 0.40              |
| 2:M8:180:ALA:O       | 2:M8:184:GLY:HA3     | 2.21                     | 0.40              |
| 2:M8:517:PRO:HB2     | 2:M8:519:TYR:CE1     | 2.57                     | 0.40              |
| 2:M8:624:ASP:OD1     | 2:M8:624:ASP:N       | 2.50                     | 0.40              |
| 2:M8:761:PRO:C       | 2:M8:763:ASP:H       | 2.30                     | 0.40              |
| 1:R16:1156:GLU:OE2   | 1:R16:1156:GLU:CA    | 2.69                     | 0.40              |
| 2:M16:783:TRP:HB3    | 2:M16:787:LEU:HG     | 2.02                     | 0.40              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 3:N16:176:VAL:HG12  | 3:N16:178:LYS:HG3    | 2.04                     | 0.40              |
| 3:N16:301:GLU:HA    | 3:N16:302:PRO:HD3    | 1.91                     | 0.40              |
| 5:P:262:ASP:OD1     | 5:P:262:ASP:N        | 2.52                     | 0.40              |
| 7:Q:229:ILE:O       | 7:Q:247:GLY:HA3      | 2.21                     | 0.40              |
| 5:P8:484:ALA:HB2    | 5:P8:519:TYR:CE1     | 2.57                     | 0.40              |
| 7:Q8:314:LEU:HB3    | 7:Q8:327:LEU:HB2     | 2.04                     | 0.40              |
| 7:Q16:259:TRP:CD1   | 7:Q16:259:TRP:N      | 2.89                     | 0.40              |
| 9:K:998:GLN:OE1     | 9:K:1001:LYS:HD2     | 2.22                     | 0.40              |
| 9:K:1055:THR:C      | 9:K:1057:GLU:N       | 2.79                     | 0.40              |
| 9:K:1074:ARG:CD     | 9:K:1126:LEU:HD22    | 2.43                     | 0.40              |
| 9:K8:955:TYR:OH     | 9:K8:984:GLY:HA2     | 2.22                     | 0.40              |
| 9:K8:1281:SER:O     | 9:K8:1283:PRO:HD3    | 2.21                     | 0.40              |
| 10:C16:747:LYS:HB3  | 10:C16:748:ALA:H     | 1.68                     | 0.40              |
| 10:C16:1507:LEU:C   | 10:C16:1509:SER:N    | 2.67                     | 0.40              |
| 10:C16:1593:TRP:CE2 | 10:C16:1603:PHE:HD2  | 2.37                     | 0.40              |
| 10:C16:1688:ARG:CG  | 23:J32:735:LYS:HE2   | 2.35                     | 0.40              |
| 11:A24:500:ASP:CG   | 11:A24:503:VAL:HG23  | 2.46                     | 0.40              |
| 10:C24:320:TRP:NE1  | 10:C24:324:LEU:HD11  | 2.36                     | 0.40              |
| 10:C24:620:PRO:HB3  | 10:C24:636:VAL:HG13  | 1.58                     | 0.40              |
| 10:C24:1003:PRO:O   | 10:C24:1012:ARG:NH1  | 2.52                     | 0.40              |
| 10:C24:1304:VAL:CG1 | 10:C24:1384:ILE:HD11 | 2.45                     | 0.40              |
| 10:C24:1812:GLU:CG  | 10:C24:1819:LEU:HD12 | 2.50                     | 0.40              |
| 11:A40:237:LEU:C    | 11:A40:239:ALA:N     | 2.79                     | 0.40              |
| 12:A:634:ILE:HD12   | 12:A:678:LYS:NZ      | 2.36                     | 0.40              |
| 13:V:925:ILE:CD1    | 14:W:801:ALA:CB      | 2.97                     | 0.40              |
| 10:C:73:ASP:OD1     | 10:C:76:ASP:CG       | 2.65                     | 0.40              |
| 10:C:275:ALA:HB1    | 10:C:326:LEU:HD13    | 2.03                     | 0.40              |
| 10:C:657:ILE:HG13   | 10:C:690:LEU:HD13    | 2.04                     | 0.40              |
| 10:C8:73:ASP:OD1    | 10:C8:76:ASP:CG      | 2.65                     | 0.40              |
| 10:C8:168:ARG:HH12  | 10:C8:229:PRO:CA     | 2.31                     | 0.40              |
| 10:C8:971:ASP:HA    | 10:C8:972:PRO:HD3    | 1.89                     | 0.40              |
| 10:C8:1756:LEU:HD11 | 10:C8:1815:VAL:CG1   | 2.51                     | 0.40              |
| 11:A16:212:LYS:HG2  | 11:A16:588:GLU:HG3   | 2.04                     | 0.40              |
| 11:A16:237:LEU:C    | 11:A16:239:ALA:N     | 2.79                     | 0.40              |
| 11:A16:787:ASP:HA   | 11:A16:788:PRO:HD3   | 1.86                     | 0.40              |
| 11:A32:650:GLY:HA2  | 11:A32:659:ARG:NH2   | 2.36                     | 0.40              |
| 18:B:17:ASP:OD1     | 18:B:17:ASP:N        | 2.55                     | 0.40              |
| 18:B:864:LEU:HB3    | 18:B:910:TYR:CZ      | 2.56                     | 0.40              |
| 18:B8:251:PHE:HZ    | 18:B8:267:VAL:HG11   | 1.86                     | 0.40              |
| 18:B8:438:TRP:HZ2   | 18:B8:483:VAL:HG22   | 1.86                     | 0.40              |
| 18:B8:1389:SER:O    | 18:B8:1393:LEU:HD12  | 2.21                     | 0.40              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 19:48:51:PRO:O       | 19:48:52:SER:C      | 2.46                     | 0.40              |
| 19:48:171:TRP:CH2    | 19:48:192:SER:HB2   | 2.56                     | 0.40              |
| 20:E8:341:TYR:C      | 20:E8:342:GLN:O     | 2.62                     | 0.40              |
| 20:E8:430:ALA:O      | 20:E8:432:ILE:N     | 2.55                     | 0.40              |
| 21:H:280:LEU:CD1     | 22:I:263:LEU:HD23   | 2.51                     | 0.40              |
| 21:H:291:VAL:HG13    | 23:J32:657:GLU:HG3  | 2.01                     | 0.40              |
| 21:H8:154:VAL:HG21   | 21:H8:188:ARG:HH21  | 1.86                     | 0.40              |
| 21:H24:294:PRO:HA    | 21:H24:300:ARG:NH2  | 2.36                     | 0.40              |
| 21:H24:316:ILE:O     | 21:H24:316:ILE:CG2  | 2.65                     | 0.40              |
| 21:H16:166:VAL:HG22  | 21:H16:193:LEU:HD13 | 2.03                     | 0.40              |
| 24:D:1376:VAL:HG11   | 24:D:1430:TYR:CE2   | 2.57                     | 0.40              |
| 24:D8:1296:SER:O     | 24:D8:1343:LYS:HE3  | 2.21                     | 0.40              |
| 24:D8:1330:ARG:HH11  | 24:D16:719:ARG:HB3  | 1.84                     | 0.40              |
| 10:C32:73:ASP:OD1    | 10:C32:76:ASP:CG    | 2.65                     | 0.40              |
| 10:C32:110:ARG:NH1   | 10:C32:118:LEU:HD13 | 2.28                     | 0.40              |
| 10:C32:381:ILE:HG22  | 10:C32:385:TYR:CE2  | 2.57                     | 0.40              |
| 10:C32:847:ARG:HD3   | 10:C32:903:ASN:CG   | 2.47                     | 0.40              |
| 10:C32:1686:LEU:HD12 | 10:C32:1755:LEU:HB2 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | R     | 1458/1495 (98%) | 1379 (95%) | 60 (4%) | 19 (1%)  | 9           | 42 |
| 1   | R16   | 1458/1495 (98%) | 1379 (95%) | 59 (4%) | 20 (1%)  | 9           | 40 |
| 1   | R8    | 1458/1495 (98%) | 1379 (95%) | 59 (4%) | 20 (1%)  | 9           | 40 |
| 2   | M     | 688/704 (98%)   | 650 (94%)  | 19 (3%) | 19 (3%)  | 4           | 24 |
| 2   | M16   | 688/704 (98%)   | 650 (94%)  | 19 (3%) | 19 (3%)  | 4           | 24 |
| 2   | M8    | 688/704 (98%)   | 650 (94%)  | 19 (3%) | 19 (3%)  | 4           | 24 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| 3   | N     | 300/302 (99%)    | 285 (95%)  | 12 (4%) | 3 (1%)   | 12          | 49 |
| 3   | N16   | 300/302 (99%)    | 285 (95%)  | 12 (4%) | 3 (1%)   | 12          | 49 |
| 3   | N8    | 300/302 (99%)    | 285 (95%)  | 12 (4%) | 3 (1%)   | 12          | 49 |
| 4   | T     | 682/684 (100%)   | 647 (95%)  | 29 (4%) | 6 (1%)   | 14          | 51 |
| 4   | T16   | 682/684 (100%)   | 647 (95%)  | 29 (4%) | 6 (1%)   | 14          | 51 |
| 4   | T8    | 682/684 (100%)   | 647 (95%)  | 29 (4%) | 6 (1%)   | 14          | 51 |
| 5   | P     | 700/716 (98%)    | 668 (95%)  | 15 (2%) | 17 (2%)  | 4           | 27 |
| 5   | P16   | 700/716 (98%)    | 668 (95%)  | 16 (2%) | 16 (2%)  | 5           | 28 |
| 5   | P8    | 700/716 (98%)    | 668 (95%)  | 16 (2%) | 16 (2%)  | 5           | 28 |
| 6   | O     | 299/326 (92%)    | 286 (96%)  | 5 (2%)  | 8 (3%)   | 4           | 25 |
| 6   | O16   | 299/326 (92%)    | 287 (96%)  | 4 (1%)  | 8 (3%)   | 4           | 25 |
| 6   | O8    | 299/326 (92%)    | 286 (96%)  | 5 (2%)  | 8 (3%)   | 4           | 25 |
| 7   | Q     | 359/361 (99%)    | 335 (93%)  | 15 (4%) | 9 (2%)   | 4           | 26 |
| 7   | Q16   | 359/361 (99%)    | 335 (93%)  | 15 (4%) | 9 (2%)   | 4           | 26 |
| 7   | Q8    | 359/361 (99%)    | 335 (93%)  | 15 (4%) | 9 (2%)   | 4           | 26 |
| 8   | L     | 970/977 (99%)    | 925 (95%)  | 34 (4%) | 11 (1%)  | 11          | 46 |
| 8   | L16   | 970/977 (99%)    | 925 (95%)  | 34 (4%) | 11 (1%)  | 11          | 46 |
| 8   | L8    | 970/977 (99%)    | 925 (95%)  | 34 (4%) | 11 (1%)  | 11          | 46 |
| 9   | K     | 701/709 (99%)    | 638 (91%)  | 29 (4%) | 34 (5%)  | 1           | 16 |
| 9   | K16   | 701/709 (99%)    | 663 (95%)  | 24 (3%) | 14 (2%)  | 6           | 31 |
| 9   | K8    | 701/709 (99%)    | 638 (91%)  | 29 (4%) | 34 (5%)  | 1           | 16 |
| 10  | C     | 1816/1838 (99%)  | 1681 (93%) | 64 (4%) | 71 (4%)  | 2           | 19 |
| 10  | C16   | 1836/1838 (100%) | 1693 (92%) | 69 (4%) | 74 (4%)  | 2           | 18 |
| 10  | C24   | 1836/1838 (100%) | 1693 (92%) | 69 (4%) | 74 (4%)  | 2           | 18 |
| 10  | C32   | 1836/1838 (100%) | 1693 (92%) | 68 (4%) | 75 (4%)  | 2           | 18 |
| 10  | C8    | 1781/1838 (97%)  | 1667 (94%) | 56 (3%) | 58 (3%)  | 3           | 21 |
| 11  | A16   | 812/860 (94%)    | 779 (96%)  | 17 (2%) | 16 (2%)  | 6           | 31 |
| 11  | A24   | 812/860 (94%)    | 778 (96%)  | 17 (2%) | 17 (2%)  | 5           | 30 |
| 11  | A32   | 812/860 (94%)    | 779 (96%)  | 17 (2%) | 16 (2%)  | 6           | 31 |
| 11  | A40   | 812/860 (94%)    | 778 (96%)  | 17 (2%) | 17 (2%)  | 5           | 30 |
| 12  | A     | 717/763 (94%)    | 688 (96%)  | 15 (2%) | 14 (2%)  | 6           | 31 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| 12  | A48   | 722/763 (95%)    | 693 (96%)  | 15 (2%) | 14 (2%)  | 6           | 32 |
| 13  | V     | 194/196 (99%)    | 175 (90%)  | 8 (4%)  | 11 (6%)  | 1           | 14 |
| 14  | W     | 783/810 (97%)    | 737 (94%)  | 30 (4%) | 16 (2%)  | 6           | 31 |
| 15  | J     | 183/185 (99%)    | 175 (96%)  | 3 (2%)  | 5 (3%)   | 4           | 25 |
| 16  | A8    | 61/63 (97%)      | 60 (98%)   | 0       | 1 (2%)   | 7           | 38 |
| 17  | F     | 26/28 (93%)      | 18 (69%)   | 3 (12%) | 5 (19%)  | 0           | 2  |
| 17  | F16   | 26/28 (93%)      | 18 (69%)   | 3 (12%) | 5 (19%)  | 0           | 2  |
| 17  | F24   | 26/28 (93%)      | 18 (69%)   | 3 (12%) | 5 (19%)  | 0           | 2  |
| 17  | F8    | 26/28 (93%)      | 18 (69%)   | 3 (12%) | 5 (19%)  | 0           | 2  |
| 18  | B     | 1963/1965 (100%) | 1806 (92%) | 79 (4%) | 78 (4%)  | 2           | 18 |
| 18  | B8    | 1963/1965 (100%) | 1807 (92%) | 78 (4%) | 78 (4%)  | 2           | 18 |
| 19  | 4     | 445/447 (100%)   | 403 (91%)  | 16 (4%) | 26 (6%)  | 1           | 14 |
| 19  | 48    | 445/447 (100%)   | 403 (91%)  | 16 (4%) | 26 (6%)  | 1           | 14 |
| 20  | E     | 517/519 (100%)   | 471 (91%)  | 19 (4%) | 27 (5%)  | 1           | 15 |
| 20  | E8    | 517/519 (100%)   | 471 (91%)  | 18 (4%) | 28 (5%)  | 1           | 15 |
| 21  | H     | 252/254 (99%)    | 245 (97%)  | 1 (0%)  | 6 (2%)   | 4           | 27 |
| 21  | H16   | 252/254 (99%)    | 245 (97%)  | 1 (0%)  | 6 (2%)   | 4           | 27 |
| 21  | H24   | 252/254 (99%)    | 245 (97%)  | 1 (0%)  | 6 (2%)   | 4           | 27 |
| 21  | H8    | 252/254 (99%)    | 245 (97%)  | 1 (0%)  | 6 (2%)   | 4           | 27 |
| 22  | I     | 233/237 (98%)    | 224 (96%)  | 7 (3%)  | 2 (1%)   | 14          | 51 |
| 22  | I16   | 233/237 (98%)    | 224 (96%)  | 7 (3%)  | 2 (1%)   | 14          | 51 |
| 22  | I24   | 233/237 (98%)    | 224 (96%)  | 7 (3%)  | 2 (1%)   | 14          | 51 |
| 22  | I8    | 233/237 (98%)    | 224 (96%)  | 7 (3%)  | 2 (1%)   | 14          | 51 |
| 23  | J16   | 195/197 (99%)    | 188 (96%)  | 5 (3%)  | 2 (1%)   | 12          | 49 |
| 23  | J24   | 195/197 (99%)    | 188 (96%)  | 5 (3%)  | 2 (1%)   | 12          | 49 |
| 23  | J32   | 195/197 (99%)    | 188 (96%)  | 5 (3%)  | 2 (1%)   | 12          | 49 |
| 23  | J8    | 195/197 (99%)    | 188 (96%)  | 5 (3%)  | 2 (1%)   | 12          | 49 |
| 24  | D     | 1447/1464 (99%)  | 1335 (92%) | 70 (5%) | 42 (3%)  | 3           | 23 |
| 24  | D16   | 1447/1464 (99%)  | 1336 (92%) | 69 (5%) | 42 (3%)  | 3           | 23 |
| 24  | D24   | 1447/1464 (99%)  | 1334 (92%) | 71 (5%) | 42 (3%)  | 3           | 23 |
| 24  | D32   | 1447/1464 (99%)  | 1334 (92%) | 71 (5%) | 42 (3%)  | 3           | 23 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|-----------|-------------|----|
| 24  | D40   | 1447/1464 (99%)   | 1336 (92%)  | 69 (5%)   | 42 (3%)   | 3           | 23 |
| 24  | D8    | 1447/1464 (99%)   | 1336 (92%)  | 69 (5%)   | 42 (3%)   | 3           | 23 |
| All | All   | 50840/51742 (98%) | 47606 (94%) | 1822 (4%) | 1412 (3%) | 6           | 24 |

All (1412) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R     | 302  | MET  |
| 1   | R     | 1183 | GLU  |
| 1   | R     | 1185 | THR  |
| 1   | R     | 1186 | THR  |
| 1   | R     | 1192 | LYS  |
| 1   | R     | 1205 | ASP  |
| 1   | R     | 1208 | LYS  |
| 1   | R     | 1210 | GLU  |
| 1   | R     | 1382 | LYS  |
| 2   | M     | 342  | VAL  |
| 2   | M     | 346  | VAL  |
| 2   | M     | 347  | LYS  |
| 2   | M     | 349  | ASP  |
| 2   | M     | 350  | SER  |
| 2   | M     | 352  | LYS  |
| 2   | M     | 756  | MET  |
| 2   | M     | 759  | LEU  |
| 2   | M     | 762  | LEU  |
| 1   | R8    | 302  | MET  |
| 1   | R8    | 1183 | GLU  |
| 1   | R8    | 1185 | THR  |
| 1   | R8    | 1186 | THR  |
| 1   | R8    | 1192 | LYS  |
| 1   | R8    | 1205 | ASP  |
| 1   | R8    | 1208 | LYS  |
| 1   | R8    | 1210 | GLU  |
| 1   | R8    | 1382 | LYS  |
| 2   | M8    | 342  | VAL  |
| 2   | M8    | 346  | VAL  |
| 2   | M8    | 347  | LYS  |
| 2   | M8    | 349  | ASP  |
| 2   | M8    | 350  | SER  |
| 2   | M8    | 352  | LYS  |
| 2   | M8    | 756  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M8    | 759  | LEU  |
| 2   | M8    | 762  | LEU  |
| 1   | R16   | 302  | MET  |
| 1   | R16   | 1183 | GLU  |
| 1   | R16   | 1185 | THR  |
| 1   | R16   | 1186 | THR  |
| 1   | R16   | 1192 | LYS  |
| 1   | R16   | 1205 | ASP  |
| 1   | R16   | 1208 | LYS  |
| 1   | R16   | 1210 | GLU  |
| 1   | R16   | 1382 | LYS  |
| 2   | M16   | 342  | VAL  |
| 2   | M16   | 346  | VAL  |
| 2   | M16   | 347  | LYS  |
| 2   | M16   | 349  | ASP  |
| 2   | M16   | 350  | SER  |
| 2   | M16   | 352  | LYS  |
| 2   | M16   | 756  | MET  |
| 2   | M16   | 759  | LEU  |
| 2   | M16   | 762  | LEU  |
| 4   | T     | 2    | ASP  |
| 4   | T8    | 2    | ASP  |
| 4   | T16   | 2    | ASP  |
| 5   | P     | 5    | SER  |
| 5   | P     | 6    | SER  |
| 5   | P     | 7    | GLU  |
| 5   | P     | 13   | LEU  |
| 5   | P     | 20   | GLU  |
| 5   | P     | 146  | SER  |
| 5   | P     | 394  | ASN  |
| 5   | P     | 395  | THR  |
| 5   | P     | 593  | GLN  |
| 5   | P     | 596  | GLY  |
| 6   | O     | 162  | THR  |
| 6   | O     | 178  | MET  |
| 6   | O     | 181  | GLU  |
| 7   | Q     | 90   | GLY  |
| 7   | Q     | 91   | GLY  |
| 7   | Q     | 223  | GLN  |
| 7   | Q     | 296  | ASN  |
| 7   | Q     | 299  | SER  |
| 5   | P8    | 5    | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | P8    | 6    | SER  |
| 5   | P8    | 7    | GLU  |
| 5   | P8    | 13   | LEU  |
| 5   | P8    | 20   | GLU  |
| 5   | P8    | 146  | SER  |
| 5   | P8    | 394  | ASN  |
| 5   | P8    | 395  | THR  |
| 5   | P8    | 593  | GLN  |
| 5   | P8    | 596  | GLY  |
| 6   | O8    | 162  | THR  |
| 6   | O8    | 178  | MET  |
| 6   | O8    | 181  | GLU  |
| 7   | Q8    | 90   | GLY  |
| 7   | Q8    | 91   | GLY  |
| 7   | Q8    | 223  | GLN  |
| 7   | Q8    | 296  | ASN  |
| 7   | Q8    | 299  | SER  |
| 5   | P16   | 5    | SER  |
| 5   | P16   | 6    | SER  |
| 5   | P16   | 7    | GLU  |
| 5   | P16   | 13   | LEU  |
| 5   | P16   | 20   | GLU  |
| 5   | P16   | 146  | SER  |
| 5   | P16   | 394  | ASN  |
| 5   | P16   | 395  | THR  |
| 5   | P16   | 593  | GLN  |
| 5   | P16   | 596  | GLY  |
| 6   | O16   | 162  | THR  |
| 6   | O16   | 178  | MET  |
| 6   | O16   | 181  | GLU  |
| 7   | Q16   | 90   | GLY  |
| 7   | Q16   | 91   | GLY  |
| 7   | Q16   | 223  | GLN  |
| 7   | Q16   | 296  | ASN  |
| 7   | Q16   | 299  | SER  |
| 8   | L     | 481  | SER  |
| 8   | L8    | 481  | SER  |
| 8   | L16   | 481  | SER  |
| 9   | K     | 728  | GLN  |
| 9   | K     | 729  | VAL  |
| 9   | K     | 892  | GLU  |
| 9   | K     | 1047 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | K     | 1048 | GLN  |
| 9   | K     | 1051 | GLU  |
| 9   | K     | 1052 | SER  |
| 9   | K     | 1054 | THR  |
| 9   | K     | 1065 | GLU  |
| 9   | K     | 1066 | ASP  |
| 9   | K     | 1067 | VAL  |
| 9   | K     | 1089 | LYS  |
| 9   | K     | 1271 | GLU  |
| 9   | K     | 1273 | GLU  |
| 9   | K     | 1278 | GLU  |
| 9   | K8    | 728  | GLN  |
| 9   | K8    | 729  | VAL  |
| 9   | K8    | 892  | GLU  |
| 9   | K8    | 1047 | SER  |
| 9   | K8    | 1048 | GLN  |
| 9   | K8    | 1051 | GLU  |
| 9   | K8    | 1052 | SER  |
| 9   | K8    | 1054 | THR  |
| 9   | K8    | 1065 | GLU  |
| 9   | K8    | 1066 | ASP  |
| 9   | K8    | 1067 | VAL  |
| 9   | K8    | 1089 | LYS  |
| 9   | K8    | 1271 | GLU  |
| 9   | K8    | 1273 | GLU  |
| 9   | K8    | 1278 | GLU  |
| 10  | C16   | 106  | GLY  |
| 10  | C16   | 250  | GLU  |
| 10  | C16   | 252  | ASN  |
| 10  | C16   | 281  | ASP  |
| 10  | C16   | 283  | SER  |
| 10  | C16   | 631  | ASP  |
| 10  | C16   | 633  | SER  |
| 10  | C16   | 634  | SER  |
| 10  | C16   | 668  | ALA  |
| 10  | C16   | 730  | LEU  |
| 10  | C16   | 1055 | GLU  |
| 10  | C16   | 1056 | VAL  |
| 10  | C16   | 1063 | PRO  |
| 10  | C16   | 1065 | SER  |
| 10  | C16   | 1067 | SER  |
| 10  | C16   | 1072 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C16   | 1080 | SER  |
| 10  | C16   | 1081 | SER  |
| 10  | C16   | 1082 | ILE  |
| 10  | C16   | 1083 | SER  |
| 10  | C16   | 1112 | LEU  |
| 10  | C16   | 1128 | SER  |
| 10  | C16   | 1130 | SER  |
| 10  | C16   | 1167 | PHE  |
| 10  | C16   | 1170 | VAL  |
| 10  | C16   | 1274 | ALA  |
| 10  | C16   | 1275 | LEU  |
| 10  | C16   | 1336 | ALA  |
| 10  | C16   | 1337 | LEU  |
| 10  | C16   | 1353 | ASP  |
| 10  | C16   | 1356 | ASP  |
| 10  | C16   | 1357 | LEU  |
| 10  | C16   | 1359 | ILE  |
| 10  | C16   | 1508 | GLN  |
| 10  | C16   | 1510 | ASP  |
| 10  | C16   | 1543 | GLU  |
| 10  | C16   | 1617 | ALA  |
| 10  | C16   | 1620 | ILE  |
| 10  | C16   | 1622 | SER  |
| 10  | C16   | 1661 | LEU  |
| 10  | C16   | 1662 | ASP  |
| 10  | C16   | 1664 | SER  |
| 11  | A24   | 55   | GLU  |
| 11  | A24   | 57   | PRO  |
| 11  | A24   | 159  | LYS  |
| 11  | A24   | 241  | VAL  |
| 11  | A24   | 463  | GLY  |
| 11  | A24   | 469  | VAL  |
| 11  | A24   | 472  | ASP  |
| 11  | A24   | 552  | GLY  |
| 11  | A24   | 556  | LYS  |
| 10  | C24   | 106  | GLY  |
| 10  | C24   | 250  | GLU  |
| 10  | C24   | 252  | ASN  |
| 10  | C24   | 281  | ASP  |
| 10  | C24   | 283  | SER  |
| 10  | C24   | 631  | ASP  |
| 10  | C24   | 633  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C24   | 634  | SER  |
| 10  | C24   | 668  | ALA  |
| 10  | C24   | 730  | LEU  |
| 10  | C24   | 1055 | GLU  |
| 10  | C24   | 1056 | VAL  |
| 10  | C24   | 1063 | PRO  |
| 10  | C24   | 1065 | SER  |
| 10  | C24   | 1067 | SER  |
| 10  | C24   | 1072 | ASP  |
| 10  | C24   | 1080 | SER  |
| 10  | C24   | 1081 | SER  |
| 10  | C24   | 1082 | ILE  |
| 10  | C24   | 1083 | SER  |
| 10  | C24   | 1112 | LEU  |
| 10  | C24   | 1128 | SER  |
| 10  | C24   | 1130 | SER  |
| 10  | C24   | 1167 | PHE  |
| 10  | C24   | 1170 | VAL  |
| 10  | C24   | 1274 | ALA  |
| 10  | C24   | 1275 | LEU  |
| 10  | C24   | 1336 | ALA  |
| 10  | C24   | 1337 | LEU  |
| 10  | C24   | 1353 | ASP  |
| 10  | C24   | 1356 | ASP  |
| 10  | C24   | 1357 | LEU  |
| 10  | C24   | 1359 | ILE  |
| 10  | C24   | 1508 | GLN  |
| 10  | C24   | 1510 | ASP  |
| 10  | C24   | 1543 | GLU  |
| 10  | C24   | 1617 | ALA  |
| 10  | C24   | 1620 | ILE  |
| 10  | C24   | 1622 | SER  |
| 10  | C24   | 1661 | LEU  |
| 10  | C24   | 1662 | ASP  |
| 10  | C24   | 1664 | SER  |
| 11  | A40   | 55   | GLU  |
| 11  | A40   | 57   | PRO  |
| 11  | A40   | 159  | LYS  |
| 11  | A40   | 241  | VAL  |
| 11  | A40   | 463  | GLY  |
| 11  | A40   | 469  | VAL  |
| 11  | A40   | 472  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A40   | 552  | GLY  |
| 11  | A40   | 556  | LYS  |
| 11  | A40   | 795  | ALA  |
| 12  | A     | 159  | LYS  |
| 12  | A     | 241  | VAL  |
| 12  | A     | 463  | GLY  |
| 12  | A     | 469  | VAL  |
| 12  | A     | 472  | ASP  |
| 12  | A     | 552  | GLY  |
| 12  | A     | 556  | LYS  |
| 12  | A     | 795  | ALA  |
| 13  | V     | 878  | ALA  |
| 13  | V     | 879  | ARG  |
| 13  | V     | 885  | ARG  |
| 14  | W     | 309  | GLU  |
| 14  | W     | 426  | SER  |
| 14  | W     | 704  | THR  |
| 15  | J     | 678  | GLY  |
| 15  | J     | 679  | GLU  |
| 15  | J     | 683  | ILE  |
| 10  | C     | 106  | GLY  |
| 10  | C     | 250  | GLU  |
| 10  | C     | 252  | ASN  |
| 10  | C     | 281  | ASP  |
| 10  | C     | 283  | SER  |
| 10  | C     | 631  | ASP  |
| 10  | C     | 633  | SER  |
| 10  | C     | 634  | SER  |
| 10  | C     | 668  | ALA  |
| 10  | C     | 730  | LEU  |
| 10  | C     | 1055 | GLU  |
| 10  | C     | 1056 | VAL  |
| 10  | C     | 1063 | PRO  |
| 10  | C     | 1065 | SER  |
| 10  | C     | 1067 | SER  |
| 10  | C     | 1072 | ASP  |
| 10  | C     | 1080 | SER  |
| 10  | C     | 1081 | SER  |
| 10  | C     | 1082 | ILE  |
| 10  | C     | 1083 | SER  |
| 10  | C     | 1112 | LEU  |
| 10  | C     | 1128 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C     | 1130 | SER  |
| 10  | C     | 1167 | PHE  |
| 10  | C     | 1170 | VAL  |
| 10  | C     | 1274 | ALA  |
| 10  | C     | 1275 | LEU  |
| 10  | C     | 1336 | ALA  |
| 10  | C     | 1337 | LEU  |
| 10  | C     | 1353 | ASP  |
| 10  | C     | 1356 | ASP  |
| 10  | C     | 1357 | LEU  |
| 10  | C     | 1359 | ILE  |
| 10  | C     | 1508 | GLN  |
| 10  | C     | 1510 | ASP  |
| 10  | C     | 1617 | ALA  |
| 10  | C     | 1620 | ILE  |
| 10  | C     | 1622 | SER  |
| 10  | C     | 1661 | LEU  |
| 10  | C     | 1662 | ASP  |
| 10  | C     | 1664 | SER  |
| 10  | C8    | 106  | GLY  |
| 10  | C8    | 250  | GLU  |
| 10  | C8    | 252  | ASN  |
| 10  | C8    | 281  | ASP  |
| 10  | C8    | 283  | SER  |
| 10  | C8    | 668  | ALA  |
| 10  | C8    | 1055 | GLU  |
| 10  | C8    | 1056 | VAL  |
| 10  | C8    | 1063 | PRO  |
| 10  | C8    | 1065 | SER  |
| 10  | C8    | 1067 | SER  |
| 10  | C8    | 1072 | ASP  |
| 10  | C8    | 1080 | SER  |
| 10  | C8    | 1081 | SER  |
| 10  | C8    | 1082 | ILE  |
| 10  | C8    | 1083 | SER  |
| 10  | C8    | 1112 | LEU  |
| 10  | C8    | 1128 | SER  |
| 10  | C8    | 1130 | SER  |
| 10  | C8    | 1167 | PHE  |
| 10  | C8    | 1170 | VAL  |
| 10  | C8    | 1274 | ALA  |
| 10  | C8    | 1275 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 1336 | ALA  |
| 10  | C8    | 1337 | LEU  |
| 10  | C8    | 1353 | ASP  |
| 10  | C8    | 1356 | ASP  |
| 10  | C8    | 1357 | LEU  |
| 10  | C8    | 1359 | ILE  |
| 10  | C8    | 1508 | GLN  |
| 10  | C8    | 1510 | ASP  |
| 10  | C8    | 1543 | GLU  |
| 10  | C8    | 1617 | ALA  |
| 10  | C8    | 1620 | ILE  |
| 10  | C8    | 1622 | SER  |
| 16  | A8    | 159  | LYS  |
| 11  | A16   | 55   | GLU  |
| 11  | A16   | 57   | PRO  |
| 11  | A16   | 241  | VAL  |
| 11  | A16   | 463  | GLY  |
| 11  | A16   | 469  | VAL  |
| 11  | A16   | 472  | ASP  |
| 11  | A16   | 552  | GLY  |
| 11  | A16   | 556  | LYS  |
| 11  | A16   | 795  | ALA  |
| 17  | F8    | 72   | SER  |
| 17  | F8    | 75   | ALA  |
| 17  | F     | 72   | SER  |
| 17  | F     | 75   | ALA  |
| 11  | A32   | 55   | GLU  |
| 11  | A32   | 57   | PRO  |
| 11  | A32   | 241  | VAL  |
| 11  | A32   | 463  | GLY  |
| 11  | A32   | 469  | VAL  |
| 11  | A32   | 472  | ASP  |
| 11  | A32   | 552  | GLY  |
| 11  | A32   | 556  | LYS  |
| 17  | F24   | 72   | SER  |
| 17  | F24   | 75   | ALA  |
| 17  | F16   | 72   | SER  |
| 17  | F16   | 75   | ALA  |
| 18  | B     | 123  | LEU  |
| 18  | B     | 125  | GLN  |
| 18  | B     | 509  | SER  |
| 18  | B     | 613  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B     | 615  | GLU  |
| 18  | B     | 616  | SER  |
| 18  | B     | 618  | VAL  |
| 18  | B     | 673  | SER  |
| 18  | B     | 674  | CYS  |
| 18  | B     | 679  | ASP  |
| 18  | B     | 681  | GLY  |
| 18  | B     | 684  | ILE  |
| 18  | B     | 685  | SER  |
| 18  | B     | 686  | LEU  |
| 18  | B     | 689  | SER  |
| 18  | B     | 690  | TRP  |
| 18  | B     | 908  | GLN  |
| 18  | B     | 981  | GLN  |
| 18  | B     | 984  | LYS  |
| 18  | B     | 987  | SER  |
| 18  | B     | 990  | PRO  |
| 18  | B     | 991  | ASP  |
| 18  | B     | 992  | TRP  |
| 18  | B     | 993  | ALA  |
| 18  | B     | 994  | CYS  |
| 18  | B     | 1066 | ASP  |
| 18  | B     | 1068 | THR  |
| 18  | B     | 1069 | VAL  |
| 18  | B     | 1117 | THR  |
| 18  | B     | 1123 | ASN  |
| 18  | B     | 1125 | VAL  |
| 18  | B     | 1129 | LYS  |
| 18  | B     | 1130 | LEU  |
| 18  | B     | 1131 | THR  |
| 18  | B     | 1134 | ALA  |
| 18  | B     | 1288 | GLY  |
| 18  | B     | 1364 | GLU  |
| 18  | B     | 1365 | ARG  |
| 18  | B     | 1595 | ASP  |
| 18  | B     | 1596 | GLY  |
| 18  | B     | 1679 | ARG  |
| 18  | B     | 1680 | SER  |
| 18  | B     | 1802 | ASP  |
| 18  | B     | 1803 | THR  |
| 18  | B8    | 123  | LEU  |
| 18  | B8    | 125  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B8    | 509  | SER  |
| 18  | B8    | 613  | LYS  |
| 18  | B8    | 615  | GLU  |
| 18  | B8    | 616  | SER  |
| 18  | B8    | 618  | VAL  |
| 18  | B8    | 673  | SER  |
| 18  | B8    | 674  | CYS  |
| 18  | B8    | 679  | ASP  |
| 18  | B8    | 681  | GLY  |
| 18  | B8    | 684  | ILE  |
| 18  | B8    | 685  | SER  |
| 18  | B8    | 686  | LEU  |
| 18  | B8    | 689  | SER  |
| 18  | B8    | 690  | TRP  |
| 18  | B8    | 908  | GLN  |
| 18  | B8    | 981  | GLN  |
| 18  | B8    | 984  | LYS  |
| 18  | B8    | 987  | SER  |
| 18  | B8    | 990  | PRO  |
| 18  | B8    | 991  | ASP  |
| 18  | B8    | 992  | TRP  |
| 18  | B8    | 993  | ALA  |
| 18  | B8    | 994  | CYS  |
| 18  | B8    | 1066 | ASP  |
| 18  | B8    | 1068 | THR  |
| 18  | B8    | 1069 | VAL  |
| 18  | B8    | 1117 | THR  |
| 18  | B8    | 1123 | ASN  |
| 18  | B8    | 1125 | VAL  |
| 18  | B8    | 1129 | LYS  |
| 18  | B8    | 1130 | LEU  |
| 18  | B8    | 1131 | THR  |
| 18  | B8    | 1134 | ALA  |
| 18  | B8    | 1288 | GLY  |
| 18  | B8    | 1364 | GLU  |
| 18  | B8    | 1365 | ARG  |
| 18  | B8    | 1595 | ASP  |
| 18  | B8    | 1596 | GLY  |
| 18  | B8    | 1679 | ARG  |
| 18  | B8    | 1680 | SER  |
| 18  | B8    | 1802 | ASP  |
| 18  | B8    | 1803 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | 4     | 51  | PRO  |
| 19  | 4     | 52  | SER  |
| 19  | 4     | 53  | SER  |
| 19  | 4     | 54  | LEU  |
| 19  | 4     | 55  | GLN  |
| 19  | 4     | 56  | GLU  |
| 19  | 4     | 57  | ASN  |
| 19  | 4     | 58  | GLU  |
| 19  | 4     | 60  | GLN  |
| 19  | 4     | 63  | GLY  |
| 19  | 4     | 65  | LYS  |
| 19  | 4     | 66  | ALA  |
| 19  | 4     | 93  | ASP  |
| 19  | 4     | 101 | ASP  |
| 19  | 4     | 188 | ALA  |
| 19  | 4     | 189 | LEU  |
| 20  | E     | 39  | SER  |
| 20  | E     | 202 | ASP  |
| 20  | E     | 203 | TRP  |
| 20  | E     | 207 | LEU  |
| 20  | E     | 340 | GLY  |
| 20  | E     | 342 | GLN  |
| 20  | E     | 348 | PRO  |
| 20  | E     | 351 | SER  |
| 20  | E     | 419 | ASN  |
| 20  | E     | 429 | PRO  |
| 20  | E     | 433 | LYS  |
| 20  | E     | 435 | ALA  |
| 20  | E     | 439 | MET  |
| 20  | E     | 441 | ARG  |
| 20  | E     | 443 | ASP  |
| 20  | E     | 444 | VAL  |
| 19  | 48    | 51  | PRO  |
| 19  | 48    | 52  | SER  |
| 19  | 48    | 53  | SER  |
| 19  | 48    | 54  | LEU  |
| 19  | 48    | 55  | GLN  |
| 19  | 48    | 56  | GLU  |
| 19  | 48    | 57  | ASN  |
| 19  | 48    | 58  | GLU  |
| 19  | 48    | 60  | GLN  |
| 19  | 48    | 63  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 19  | 48    | 65   | LYS  |
| 19  | 48    | 66   | ALA  |
| 19  | 48    | 93   | ASP  |
| 19  | 48    | 101  | ASP  |
| 19  | 48    | 188  | ALA  |
| 19  | 48    | 189  | LEU  |
| 20  | E8    | 39   | SER  |
| 20  | E8    | 202  | ASP  |
| 20  | E8    | 203  | TRP  |
| 20  | E8    | 207  | LEU  |
| 20  | E8    | 340  | GLY  |
| 20  | E8    | 342  | GLN  |
| 20  | E8    | 348  | PRO  |
| 20  | E8    | 351  | SER  |
| 20  | E8    | 419  | ASN  |
| 20  | E8    | 429  | PRO  |
| 20  | E8    | 433  | LYS  |
| 20  | E8    | 435  | ALA  |
| 20  | E8    | 439  | MET  |
| 20  | E8    | 441  | ARG  |
| 20  | E8    | 443  | ASP  |
| 20  | E8    | 444  | VAL  |
| 21  | H     | 320  | SER  |
| 22  | I     | 297  | HIS  |
| 23  | J32   | 680  | LEU  |
| 21  | H8    | 320  | SER  |
| 22  | I8    | 297  | HIS  |
| 23  | J8    | 680  | LEU  |
| 21  | H24   | 320  | SER  |
| 22  | I24   | 297  | HIS  |
| 23  | J24   | 680  | LEU  |
| 21  | H16   | 320  | SER  |
| 22  | I16   | 297  | HIS  |
| 23  | J16   | 680  | LEU  |
| 24  | D     | 451  | SER  |
| 24  | D     | 746  | ALA  |
| 24  | D     | 758  | ALA  |
| 24  | D     | 760  | SER  |
| 24  | D     | 765  | SER  |
| 24  | D     | 1062 | GLN  |
| 24  | D     | 1067 | SER  |
| 24  | D     | 1068 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D     | 1075 | HIS  |
| 24  | D     | 1403 | LEU  |
| 24  | D8    | 746  | ALA  |
| 24  | D8    | 758  | ALA  |
| 24  | D8    | 760  | SER  |
| 24  | D8    | 765  | SER  |
| 24  | D8    | 1062 | GLN  |
| 24  | D8    | 1067 | SER  |
| 24  | D8    | 1068 | THR  |
| 24  | D8    | 1075 | HIS  |
| 24  | D8    | 1403 | LEU  |
| 24  | D16   | 451  | SER  |
| 24  | D16   | 746  | ALA  |
| 24  | D16   | 758  | ALA  |
| 24  | D16   | 760  | SER  |
| 24  | D16   | 765  | SER  |
| 24  | D16   | 1062 | GLN  |
| 24  | D16   | 1067 | SER  |
| 24  | D16   | 1068 | THR  |
| 24  | D16   | 1075 | HIS  |
| 24  | D16   | 1403 | LEU  |
| 24  | D24   | 746  | ALA  |
| 24  | D24   | 758  | ALA  |
| 24  | D24   | 760  | SER  |
| 24  | D24   | 765  | SER  |
| 24  | D24   | 1062 | GLN  |
| 24  | D24   | 1067 | SER  |
| 24  | D24   | 1068 | THR  |
| 24  | D24   | 1075 | HIS  |
| 24  | D24   | 1403 | LEU  |
| 24  | D32   | 451  | SER  |
| 24  | D32   | 746  | ALA  |
| 24  | D32   | 758  | ALA  |
| 24  | D32   | 760  | SER  |
| 24  | D32   | 765  | SER  |
| 24  | D32   | 1062 | GLN  |
| 24  | D32   | 1067 | SER  |
| 24  | D32   | 1068 | THR  |
| 24  | D32   | 1075 | HIS  |
| 24  | D32   | 1403 | LEU  |
| 24  | D40   | 451  | SER  |
| 24  | D40   | 746  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D40   | 758  | ALA  |
| 24  | D40   | 760  | SER  |
| 24  | D40   | 765  | SER  |
| 24  | D40   | 1062 | GLN  |
| 24  | D40   | 1067 | SER  |
| 24  | D40   | 1068 | THR  |
| 24  | D40   | 1075 | HIS  |
| 24  | D40   | 1403 | LEU  |
| 10  | C32   | 106  | GLY  |
| 10  | C32   | 250  | GLU  |
| 10  | C32   | 252  | ASN  |
| 10  | C32   | 281  | ASP  |
| 10  | C32   | 283  | SER  |
| 10  | C32   | 631  | ASP  |
| 10  | C32   | 633  | SER  |
| 10  | C32   | 634  | SER  |
| 10  | C32   | 668  | ALA  |
| 10  | C32   | 730  | LEU  |
| 10  | C32   | 1055 | GLU  |
| 10  | C32   | 1056 | VAL  |
| 10  | C32   | 1063 | PRO  |
| 10  | C32   | 1065 | SER  |
| 10  | C32   | 1067 | SER  |
| 10  | C32   | 1072 | ASP  |
| 10  | C32   | 1080 | SER  |
| 10  | C32   | 1081 | SER  |
| 10  | C32   | 1082 | ILE  |
| 10  | C32   | 1083 | SER  |
| 10  | C32   | 1112 | LEU  |
| 10  | C32   | 1128 | SER  |
| 10  | C32   | 1130 | SER  |
| 10  | C32   | 1167 | PHE  |
| 10  | C32   | 1170 | VAL  |
| 10  | C32   | 1274 | ALA  |
| 10  | C32   | 1275 | LEU  |
| 10  | C32   | 1336 | ALA  |
| 10  | C32   | 1337 | LEU  |
| 10  | C32   | 1353 | ASP  |
| 10  | C32   | 1356 | ASP  |
| 10  | C32   | 1357 | LEU  |
| 10  | C32   | 1359 | ILE  |
| 10  | C32   | 1508 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C32   | 1510 | ASP  |
| 10  | C32   | 1543 | GLU  |
| 10  | C32   | 1617 | ALA  |
| 10  | C32   | 1620 | ILE  |
| 10  | C32   | 1622 | SER  |
| 10  | C32   | 1661 | LEU  |
| 10  | C32   | 1662 | ASP  |
| 10  | C32   | 1664 | SER  |
| 12  | A48   | 159  | LYS  |
| 12  | A48   | 241  | VAL  |
| 12  | A48   | 463  | GLY  |
| 12  | A48   | 469  | VAL  |
| 12  | A48   | 472  | ASP  |
| 12  | A48   | 552  | GLY  |
| 12  | A48   | 556  | LYS  |
| 12  | A48   | 795  | ALA  |
| 1   | R     | 533  | GLY  |
| 1   | R     | 537  | GLU  |
| 1   | R     | 1187 | ARG  |
| 2   | M     | 157  | GLY  |
| 2   | M     | 344  | GLN  |
| 2   | M     | 348  | GLU  |
| 2   | M     | 355  | THR  |
| 2   | M     | 386  | ASN  |
| 2   | M     | 390  | TYR  |
| 2   | M     | 758  | GLU  |
| 3   | N     | 3    | GLY  |
| 3   | N     | 168  | VAL  |
| 1   | R8    | 533  | GLY  |
| 1   | R8    | 537  | GLU  |
| 1   | R8    | 1187 | ARG  |
| 2   | M8    | 157  | GLY  |
| 2   | M8    | 344  | GLN  |
| 2   | M8    | 348  | GLU  |
| 2   | M8    | 355  | THR  |
| 2   | M8    | 386  | ASN  |
| 2   | M8    | 390  | TYR  |
| 2   | M8    | 758  | GLU  |
| 3   | N8    | 3    | GLY  |
| 3   | N8    | 168  | VAL  |
| 1   | R16   | 533  | GLY  |
| 1   | R16   | 537  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R16   | 1187 | ARG  |
| 2   | M16   | 157  | GLY  |
| 2   | M16   | 344  | GLN  |
| 2   | M16   | 348  | GLU  |
| 2   | M16   | 355  | THR  |
| 2   | M16   | 386  | ASN  |
| 2   | M16   | 390  | TYR  |
| 2   | M16   | 758  | GLU  |
| 3   | N16   | 3    | GLY  |
| 3   | N16   | 168  | VAL  |
| 4   | T     | 548  | ASP  |
| 4   | T8    | 548  | ASP  |
| 4   | T16   | 548  | ASP  |
| 5   | P     | 4    | MET  |
| 5   | P     | 8    | SER  |
| 5   | P     | 10   | GLY  |
| 5   | P     | 11   | GLY  |
| 5   | P     | 144  | THR  |
| 6   | O     | 94   | GLY  |
| 6   | O     | 164  | GLY  |
| 6   | O     | 180  | GLY  |
| 7   | Q     | 89   | GLY  |
| 7   | Q     | 93   | GLY  |
| 7   | Q     | 95   | PHE  |
| 7   | Q     | 273  | GLU  |
| 5   | P8    | 4    | MET  |
| 5   | P8    | 8    | SER  |
| 5   | P8    | 10   | GLY  |
| 5   | P8    | 11   | GLY  |
| 5   | P8    | 144  | THR  |
| 6   | O8    | 94   | GLY  |
| 6   | O8    | 164  | GLY  |
| 6   | O8    | 180  | GLY  |
| 7   | Q8    | 89   | GLY  |
| 7   | Q8    | 93   | GLY  |
| 7   | Q8    | 95   | PHE  |
| 7   | Q8    | 273  | GLU  |
| 5   | P16   | 4    | MET  |
| 5   | P16   | 8    | SER  |
| 5   | P16   | 10   | GLY  |
| 5   | P16   | 11   | GLY  |
| 5   | P16   | 144  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | O16   | 94   | GLY  |
| 6   | O16   | 164  | GLY  |
| 6   | O16   | 180  | GLY  |
| 7   | Q16   | 89   | GLY  |
| 7   | Q16   | 93   | GLY  |
| 7   | Q16   | 95   | PHE  |
| 7   | Q16   | 273  | GLU  |
| 8   | L     | 966  | TYR  |
| 8   | L     | 968  | THR  |
| 8   | L     | 975  | ASP  |
| 8   | L     | 988  | LEU  |
| 8   | L8    | 966  | TYR  |
| 8   | L8    | 968  | THR  |
| 8   | L8    | 975  | ASP  |
| 8   | L8    | 988  | LEU  |
| 8   | L16   | 966  | TYR  |
| 8   | L16   | 968  | THR  |
| 8   | L16   | 975  | ASP  |
| 8   | L16   | 988  | LEU  |
| 9   | K     | 638  | TRP  |
| 9   | K     | 719  | GLY  |
| 9   | K     | 724  | GLY  |
| 9   | K     | 890  | GLU  |
| 9   | K     | 966  | ASN  |
| 9   | K     | 1140 | GLN  |
| 9   | K     | 1224 | GLY  |
| 9   | K     | 1240 | SER  |
| 9   | K     | 1282 | SER  |
| 9   | K8    | 638  | TRP  |
| 9   | K8    | 719  | GLY  |
| 9   | K8    | 724  | GLY  |
| 9   | K8    | 890  | GLU  |
| 9   | K8    | 966  | ASN  |
| 9   | K8    | 1140 | GLN  |
| 9   | K8    | 1224 | GLY  |
| 9   | K8    | 1240 | SER  |
| 9   | K8    | 1282 | SER  |
| 9   | K16   | 724  | GLY  |
| 9   | K16   | 892  | GLU  |
| 9   | K16   | 1057 | GLU  |
| 10  | C16   | 428  | GLY  |
| 10  | C16   | 622  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C16   | 624  | GLY  |
| 10  | C16   | 627  | VAL  |
| 10  | C16   | 669  | GLY  |
| 10  | C16   | 729  | SER  |
| 10  | C16   | 1075 | ASP  |
| 10  | C16   | 1078 | GLY  |
| 10  | C16   | 1079 | THR  |
| 10  | C16   | 1358 | ASP  |
| 10  | C16   | 1444 | GLY  |
| 10  | C16   | 1499 | ASN  |
| 10  | C16   | 1504 | ASP  |
| 10  | C16   | 1544 | GLY  |
| 10  | C16   | 1619 | PRO  |
| 10  | C16   | 1623 | ILE  |
| 10  | C16   | 1626 | GLN  |
| 10  | C16   | 1780 | ARG  |
| 11  | A24   | 29   | GLN  |
| 11  | A24   | 462  | THR  |
| 11  | A24   | 471  | ASN  |
| 11  | A24   | 559  | VAL  |
| 11  | A24   | 783  | PHE  |
| 11  | A24   | 795  | ALA  |
| 10  | C24   | 428  | GLY  |
| 10  | C24   | 622  | VAL  |
| 10  | C24   | 624  | GLY  |
| 10  | C24   | 627  | VAL  |
| 10  | C24   | 669  | GLY  |
| 10  | C24   | 729  | SER  |
| 10  | C24   | 1075 | ASP  |
| 10  | C24   | 1078 | GLY  |
| 10  | C24   | 1079 | THR  |
| 10  | C24   | 1358 | ASP  |
| 10  | C24   | 1444 | GLY  |
| 10  | C24   | 1499 | ASN  |
| 10  | C24   | 1504 | ASP  |
| 10  | C24   | 1619 | PRO  |
| 10  | C24   | 1623 | ILE  |
| 10  | C24   | 1626 | GLN  |
| 10  | C24   | 1780 | ARG  |
| 11  | A40   | 29   | GLN  |
| 11  | A40   | 462  | THR  |
| 11  | A40   | 471  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A40   | 559  | VAL  |
| 11  | A40   | 783  | PHE  |
| 12  | A     | 462  | THR  |
| 12  | A     | 471  | ASN  |
| 12  | A     | 559  | VAL  |
| 12  | A     | 783  | PHE  |
| 13  | V     | 877  | VAL  |
| 13  | V     | 881  | GLY  |
| 13  | V     | 883  | PRO  |
| 13  | V     | 890  | ARG  |
| 14  | W     | 345  | ALA  |
| 14  | W     | 424  | ALA  |
| 10  | C     | 428  | GLY  |
| 10  | C     | 622  | VAL  |
| 10  | C     | 624  | GLY  |
| 10  | C     | 627  | VAL  |
| 10  | C     | 669  | GLY  |
| 10  | C     | 729  | SER  |
| 10  | C     | 1075 | ASP  |
| 10  | C     | 1078 | GLY  |
| 10  | C     | 1079 | THR  |
| 10  | C     | 1358 | ASP  |
| 10  | C     | 1444 | GLY  |
| 10  | C     | 1499 | ASN  |
| 10  | C     | 1504 | ASP  |
| 10  | C     | 1619 | PRO  |
| 10  | C     | 1623 | ILE  |
| 10  | C     | 1626 | GLN  |
| 10  | C     | 1780 | ARG  |
| 10  | C8    | 428  | GLY  |
| 10  | C8    | 669  | GLY  |
| 10  | C8    | 1075 | ASP  |
| 10  | C8    | 1078 | GLY  |
| 10  | C8    | 1079 | THR  |
| 10  | C8    | 1358 | ASP  |
| 10  | C8    | 1444 | GLY  |
| 10  | C8    | 1499 | ASN  |
| 10  | C8    | 1504 | ASP  |
| 10  | C8    | 1619 | PRO  |
| 10  | C8    | 1623 | ILE  |
| 10  | C8    | 1626 | GLN  |
| 10  | C8    | 1780 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A16   | 29   | GLN  |
| 11  | A16   | 462  | THR  |
| 11  | A16   | 471  | ASN  |
| 11  | A16   | 559  | VAL  |
| 11  | A16   | 783  | PHE  |
| 17  | F8    | 70   | PRO  |
| 17  | F     | 70   | PRO  |
| 11  | A32   | 29   | GLN  |
| 11  | A32   | 462  | THR  |
| 11  | A32   | 471  | ASN  |
| 11  | A32   | 559  | VAL  |
| 11  | A32   | 783  | PHE  |
| 11  | A32   | 795  | ALA  |
| 17  | F24   | 70   | PRO  |
| 17  | F16   | 70   | PRO  |
| 18  | B     | 114  | GLY  |
| 18  | B     | 414  | GLY  |
| 18  | B     | 971  | ASP  |
| 18  | B     | 1116 | GLU  |
| 18  | B     | 1229 | GLY  |
| 18  | B     | 1280 | ASN  |
| 18  | B     | 1289 | ASP  |
| 18  | B     | 1360 | SER  |
| 18  | B     | 1363 | ALA  |
| 18  | B     | 1786 | PRO  |
| 18  | B     | 1807 | PRO  |
| 18  | B     | 1808 | GLY  |
| 18  | B8    | 114  | GLY  |
| 18  | B8    | 414  | GLY  |
| 18  | B8    | 971  | ASP  |
| 18  | B8    | 1116 | GLU  |
| 18  | B8    | 1229 | GLY  |
| 18  | B8    | 1280 | ASN  |
| 18  | B8    | 1289 | ASP  |
| 18  | B8    | 1360 | SER  |
| 18  | B8    | 1363 | ALA  |
| 18  | B8    | 1786 | PRO  |
| 18  | B8    | 1807 | PRO  |
| 18  | B8    | 1808 | GLY  |
| 19  | 4     | 92   | THR  |
| 19  | 4     | 187  | SER  |
| 19  | 4     | 295  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | E     | 434  | TRP  |
| 20  | E     | 440  | VAL  |
| 19  | 48    | 92   | THR  |
| 19  | 48    | 187  | SER  |
| 19  | 48    | 295  | SER  |
| 20  | E8    | 434  | TRP  |
| 20  | E8    | 440  | VAL  |
| 21  | H     | 317  | ALA  |
| 21  | H     | 319  | GLY  |
| 21  | H     | 322  | LEU  |
| 22  | I     | 208  | HIS  |
| 21  | H8    | 317  | ALA  |
| 21  | H8    | 319  | GLY  |
| 21  | H8    | 322  | LEU  |
| 22  | I8    | 208  | HIS  |
| 21  | H24   | 317  | ALA  |
| 21  | H24   | 319  | GLY  |
| 21  | H24   | 322  | LEU  |
| 22  | I24   | 208  | HIS  |
| 21  | H16   | 317  | ALA  |
| 21  | H16   | 319  | GLY  |
| 21  | H16   | 322  | LEU  |
| 22  | I16   | 208  | HIS  |
| 24  | D     | 218  | GLY  |
| 24  | D     | 312  | ALA  |
| 24  | D     | 361  | ILE  |
| 24  | D     | 368  | ASN  |
| 24  | D     | 397  | ALA  |
| 24  | D     | 399  | SER  |
| 24  | D     | 743  | GLU  |
| 24  | D     | 1149 | VAL  |
| 24  | D     | 1152 | ALA  |
| 24  | D     | 1402 | ILE  |
| 24  | D     | 1406 | SER  |
| 24  | D8    | 218  | GLY  |
| 24  | D8    | 312  | ALA  |
| 24  | D8    | 361  | ILE  |
| 24  | D8    | 368  | ASN  |
| 24  | D8    | 397  | ALA  |
| 24  | D8    | 399  | SER  |
| 24  | D8    | 451  | SER  |
| 24  | D8    | 743  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D8    | 1149 | VAL  |
| 24  | D8    | 1152 | ALA  |
| 24  | D8    | 1402 | ILE  |
| 24  | D8    | 1406 | SER  |
| 24  | D16   | 218  | GLY  |
| 24  | D16   | 361  | ILE  |
| 24  | D16   | 368  | ASN  |
| 24  | D16   | 397  | ALA  |
| 24  | D16   | 399  | SER  |
| 24  | D16   | 743  | GLU  |
| 24  | D16   | 1149 | VAL  |
| 24  | D16   | 1152 | ALA  |
| 24  | D16   | 1402 | ILE  |
| 24  | D16   | 1406 | SER  |
| 24  | D24   | 218  | GLY  |
| 24  | D24   | 312  | ALA  |
| 24  | D24   | 361  | ILE  |
| 24  | D24   | 368  | ASN  |
| 24  | D24   | 397  | ALA  |
| 24  | D24   | 399  | SER  |
| 24  | D24   | 451  | SER  |
| 24  | D24   | 743  | GLU  |
| 24  | D24   | 1149 | VAL  |
| 24  | D24   | 1152 | ALA  |
| 24  | D24   | 1402 | ILE  |
| 24  | D24   | 1406 | SER  |
| 24  | D32   | 218  | GLY  |
| 24  | D32   | 361  | ILE  |
| 24  | D32   | 368  | ASN  |
| 24  | D32   | 397  | ALA  |
| 24  | D32   | 399  | SER  |
| 24  | D32   | 743  | GLU  |
| 24  | D32   | 1149 | VAL  |
| 24  | D32   | 1152 | ALA  |
| 24  | D32   | 1402 | ILE  |
| 24  | D32   | 1406 | SER  |
| 24  | D40   | 218  | GLY  |
| 24  | D40   | 361  | ILE  |
| 24  | D40   | 368  | ASN  |
| 24  | D40   | 397  | ALA  |
| 24  | D40   | 399  | SER  |
| 24  | D40   | 743  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D40   | 1149 | VAL  |
| 24  | D40   | 1152 | ALA  |
| 24  | D40   | 1402 | ILE  |
| 24  | D40   | 1406 | SER  |
| 10  | C32   | 428  | GLY  |
| 10  | C32   | 622  | VAL  |
| 10  | C32   | 624  | GLY  |
| 10  | C32   | 627  | VAL  |
| 10  | C32   | 669  | GLY  |
| 10  | C32   | 729  | SER  |
| 10  | C32   | 1075 | ASP  |
| 10  | C32   | 1078 | GLY  |
| 10  | C32   | 1079 | THR  |
| 10  | C32   | 1358 | ASP  |
| 10  | C32   | 1444 | GLY  |
| 10  | C32   | 1499 | ASN  |
| 10  | C32   | 1504 | ASP  |
| 10  | C32   | 1544 | GLY  |
| 10  | C32   | 1619 | PRO  |
| 10  | C32   | 1623 | ILE  |
| 10  | C32   | 1626 | GLN  |
| 10  | C32   | 1780 | ARG  |
| 12  | A48   | 462  | THR  |
| 12  | A48   | 471  | ASN  |
| 12  | A48   | 559  | VAL  |
| 12  | A48   | 783  | PHE  |
| 1   | R     | 46   | GLU  |
| 1   | R     | 525  | GLU  |
| 1   | R     | 814  | LEU  |
| 1   | R     | 1189 | PRO  |
| 1   | R8    | 46   | GLU  |
| 1   | R8    | 525  | GLU  |
| 1   | R8    | 814  | LEU  |
| 1   | R8    | 1189 | PRO  |
| 2   | M8    | 343  | MET  |
| 1   | R16   | 46   | GLU  |
| 1   | R16   | 525  | GLU  |
| 1   | R16   | 814  | LEU  |
| 1   | R16   | 1189 | PRO  |
| 2   | M16   | 343  | MET  |
| 4   | T     | 494  | VAL  |
| 4   | T8    | 494  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | T16   | 494  | VAL  |
| 8   | L     | 973  | THR  |
| 8   | L     | 989  | THR  |
| 8   | L8    | 973  | THR  |
| 8   | L8    | 989  | THR  |
| 8   | L16   | 973  | THR  |
| 8   | L16   | 989  | THR  |
| 9   | K     | 726  | GLU  |
| 9   | K     | 1056 | VAL  |
| 9   | K     | 1063 | GLU  |
| 9   | K     | 1064 | PRO  |
| 9   | K     | 1277 | ALA  |
| 9   | K     | 1283 | PRO  |
| 9   | K8    | 726  | GLU  |
| 9   | K8    | 1056 | VAL  |
| 9   | K8    | 1063 | GLU  |
| 9   | K8    | 1064 | PRO  |
| 9   | K8    | 1277 | ALA  |
| 9   | K8    | 1283 | PRO  |
| 9   | K16   | 643  | GLY  |
| 9   | K16   | 1058 | GLU  |
| 9   | K16   | 1220 | ASN  |
| 9   | K16   | 1273 | GLU  |
| 9   | K16   | 1277 | ALA  |
| 9   | K16   | 1279 | GLU  |
| 10  | C16   | 448  | LYS  |
| 10  | C16   | 716  | THR  |
| 10  | C16   | 1061 | ASN  |
| 10  | C16   | 1103 | MET  |
| 10  | C16   | 1667 | LEU  |
| 11  | A24   | 242  | THR  |
| 10  | C24   | 448  | LYS  |
| 10  | C24   | 716  | THR  |
| 10  | C24   | 1061 | ASN  |
| 10  | C24   | 1103 | MET  |
| 10  | C24   | 1544 | GLY  |
| 10  | C24   | 1667 | LEU  |
| 11  | A40   | 242  | THR  |
| 12  | A     | 242  | THR  |
| 13  | V     | 818  | THR  |
| 13  | V     | 880  | ARG  |
| 14  | W     | 9    | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 14  | W     | 503  | LEU  |
| 14  | W     | 598  | ILE  |
| 14  | W     | 702  | PRO  |
| 15  | J     | 680  | LEU  |
| 10  | C     | 716  | THR  |
| 10  | C     | 1061 | ASN  |
| 10  | C     | 1103 | MET  |
| 10  | C     | 1667 | LEU  |
| 10  | C8    | 1061 | ASN  |
| 10  | C8    | 1103 | MET  |
| 10  | C8    | 1544 | GLY  |
| 11  | A16   | 242  | THR  |
| 17  | F8    | 71   | GLU  |
| 17  | F     | 71   | GLU  |
| 11  | A32   | 242  | THR  |
| 17  | F24   | 71   | GLU  |
| 17  | F16   | 71   | GLU  |
| 18  | B     | 250  | ASN  |
| 18  | B     | 672  | THR  |
| 18  | B     | 683  | ASN  |
| 18  | B     | 1228 | SER  |
| 18  | B     | 1681 | GLN  |
| 18  | B     | 1800 | ARG  |
| 18  | B     | 1804 | THR  |
| 18  | B8    | 250  | ASN  |
| 18  | B8    | 672  | THR  |
| 18  | B8    | 683  | ASN  |
| 18  | B8    | 1228 | SER  |
| 18  | B8    | 1681 | GLN  |
| 18  | B8    | 1800 | ARG  |
| 18  | B8    | 1804 | THR  |
| 19  | 4     | 61   | GLU  |
| 19  | 4     | 73   | LEU  |
| 19  | 4     | 91   | PRO  |
| 19  | 4     | 190  | ARG  |
| 20  | E     | 437  | SER  |
| 20  | E     | 438  | SER  |
| 19  | 48    | 61   | GLU  |
| 19  | 48    | 73   | LEU  |
| 19  | 48    | 91   | PRO  |
| 19  | 48    | 190  | ARG  |
| 20  | E8    | 437  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | E8    | 438  | SER  |
| 21  | H     | 321  | SER  |
| 21  | H     | 327  | SER  |
| 21  | H8    | 321  | SER  |
| 21  | H8    | 327  | SER  |
| 21  | H24   | 321  | SER  |
| 21  | H24   | 327  | SER  |
| 21  | H16   | 321  | SER  |
| 21  | H16   | 327  | SER  |
| 24  | D     | 302  | LYS  |
| 24  | D     | 366  | PHE  |
| 24  | D     | 370  | ARG  |
| 24  | D     | 634  | THR  |
| 24  | D     | 683  | MET  |
| 24  | D     | 761  | ASN  |
| 24  | D     | 766  | ALA  |
| 24  | D     | 1397 | THR  |
| 24  | D     | 1401 | LEU  |
| 24  | D8    | 302  | LYS  |
| 24  | D8    | 366  | PHE  |
| 24  | D8    | 370  | ARG  |
| 24  | D8    | 634  | THR  |
| 24  | D8    | 683  | MET  |
| 24  | D8    | 761  | ASN  |
| 24  | D8    | 766  | ALA  |
| 24  | D8    | 1397 | THR  |
| 24  | D8    | 1401 | LEU  |
| 24  | D16   | 302  | LYS  |
| 24  | D16   | 312  | ALA  |
| 24  | D16   | 366  | PHE  |
| 24  | D16   | 370  | ARG  |
| 24  | D16   | 634  | THR  |
| 24  | D16   | 683  | MET  |
| 24  | D16   | 761  | ASN  |
| 24  | D16   | 766  | ALA  |
| 24  | D16   | 1397 | THR  |
| 24  | D16   | 1401 | LEU  |
| 24  | D24   | 302  | LYS  |
| 24  | D24   | 366  | PHE  |
| 24  | D24   | 370  | ARG  |
| 24  | D24   | 634  | THR  |
| 24  | D24   | 683  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D24   | 761  | ASN  |
| 24  | D24   | 766  | ALA  |
| 24  | D24   | 1397 | THR  |
| 24  | D24   | 1401 | LEU  |
| 24  | D32   | 302  | LYS  |
| 24  | D32   | 312  | ALA  |
| 24  | D32   | 366  | PHE  |
| 24  | D32   | 370  | ARG  |
| 24  | D32   | 634  | THR  |
| 24  | D32   | 683  | MET  |
| 24  | D32   | 761  | ASN  |
| 24  | D32   | 766  | ALA  |
| 24  | D32   | 1397 | THR  |
| 24  | D32   | 1401 | LEU  |
| 24  | D40   | 302  | LYS  |
| 24  | D40   | 312  | ALA  |
| 24  | D40   | 366  | PHE  |
| 24  | D40   | 370  | ARG  |
| 24  | D40   | 634  | THR  |
| 24  | D40   | 683  | MET  |
| 24  | D40   | 761  | ASN  |
| 24  | D40   | 766  | ALA  |
| 24  | D40   | 1397 | THR  |
| 24  | D40   | 1401 | LEU  |
| 10  | C32   | 448  | LYS  |
| 10  | C32   | 716  | THR  |
| 10  | C32   | 1061 | ASN  |
| 10  | C32   | 1103 | MET  |
| 10  | C32   | 1667 | LEU  |
| 12  | A48   | 242  | THR  |
| 1   | R     | 51   | VAL  |
| 1   | R     | 1209 | GLY  |
| 2   | M     | 343  | MET  |
| 1   | R8    | 51   | VAL  |
| 1   | R8    | 1209 | GLY  |
| 1   | R16   | 51   | VAL  |
| 1   | R16   | 1209 | GLY  |
| 4   | T     | 313  | GLN  |
| 4   | T     | 318  | SER  |
| 4   | T8    | 313  | GLN  |
| 4   | T8    | 318  | SER  |
| 4   | T16   | 313  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | T16   | 318  | SER  |
| 6   | O     | 165  | LYS  |
| 6   | O8    | 165  | LYS  |
| 6   | O16   | 165  | LYS  |
| 8   | L     | 556  | ASN  |
| 8   | L     | 585  | ASN  |
| 8   | L     | 859  | HIS  |
| 8   | L     | 964  | ASP  |
| 8   | L8    | 556  | ASN  |
| 8   | L8    | 585  | ASN  |
| 8   | L8    | 859  | HIS  |
| 8   | L8    | 964  | ASP  |
| 8   | L16   | 556  | ASN  |
| 8   | L16   | 585  | ASN  |
| 8   | L16   | 859  | HIS  |
| 8   | L16   | 964  | ASP  |
| 9   | K     | 1139 | ILE  |
| 9   | K     | 1234 | ARG  |
| 9   | K8    | 1139 | ILE  |
| 9   | K8    | 1234 | ARG  |
| 9   | K16   | 726  | GLU  |
| 9   | K16   | 1065 | GLU  |
| 9   | K16   | 1140 | GLN  |
| 9   | K16   | 1274 | GLY  |
| 10  | C16   | 248  | LEU  |
| 10  | C16   | 447  | PHE  |
| 10  | C16   | 451  | GLU  |
| 10  | C16   | 623  | VAL  |
| 10  | C16   | 849  | SER  |
| 10  | C24   | 248  | LEU  |
| 10  | C24   | 447  | PHE  |
| 10  | C24   | 451  | GLU  |
| 10  | C24   | 623  | VAL  |
| 10  | C24   | 849  | SER  |
| 14  | W     | 11   | ALA  |
| 14  | W     | 706  | LYS  |
| 15  | J     | 688  | PRO  |
| 10  | C     | 248  | LEU  |
| 10  | C     | 451  | GLU  |
| 10  | C     | 623  | VAL  |
| 10  | C     | 849  | SER  |
| 10  | C8    | 248  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 451  | GLU  |
| 10  | C8    | 849  | SER  |
| 18  | B     | 193  | LYS  |
| 18  | B     | 501  | SER  |
| 18  | B     | 1113 | PRO  |
| 18  | B     | 1638 | SER  |
| 18  | B     | 1787 | LYS  |
| 18  | B     | 1789 | THR  |
| 18  | B8    | 193  | LYS  |
| 18  | B8    | 501  | SER  |
| 18  | B8    | 1113 | PRO  |
| 18  | B8    | 1638 | SER  |
| 18  | B8    | 1787 | LYS  |
| 18  | B8    | 1789 | THR  |
| 20  | E     | 446  | PRO  |
| 20  | E8    | 446  | PRO  |
| 24  | D     | 248  | LYS  |
| 24  | D     | 357  | SER  |
| 24  | D     | 405  | GLN  |
| 24  | D     | 408  | ASP  |
| 24  | D     | 768  | LYS  |
| 24  | D     | 770  | GLN  |
| 24  | D8    | 248  | LYS  |
| 24  | D8    | 357  | SER  |
| 24  | D8    | 405  | GLN  |
| 24  | D8    | 408  | ASP  |
| 24  | D8    | 768  | LYS  |
| 24  | D8    | 770  | GLN  |
| 24  | D16   | 248  | LYS  |
| 24  | D16   | 357  | SER  |
| 24  | D16   | 405  | GLN  |
| 24  | D16   | 408  | ASP  |
| 24  | D16   | 768  | LYS  |
| 24  | D16   | 770  | GLN  |
| 24  | D24   | 248  | LYS  |
| 24  | D24   | 357  | SER  |
| 24  | D24   | 405  | GLN  |
| 24  | D24   | 408  | ASP  |
| 24  | D24   | 768  | LYS  |
| 24  | D24   | 770  | GLN  |
| 24  | D32   | 248  | LYS  |
| 24  | D32   | 357  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D32   | 405  | GLN  |
| 24  | D32   | 408  | ASP  |
| 24  | D32   | 768  | LYS  |
| 24  | D32   | 770  | GLN  |
| 24  | D40   | 248  | LYS  |
| 24  | D40   | 357  | SER  |
| 24  | D40   | 405  | GLN  |
| 24  | D40   | 408  | ASP  |
| 24  | D40   | 768  | LYS  |
| 24  | D40   | 770  | GLN  |
| 10  | C32   | 248  | LEU  |
| 10  | C32   | 447  | PHE  |
| 10  | C32   | 451  | GLU  |
| 10  | C32   | 623  | VAL  |
| 10  | C32   | 849  | SER  |
| 1   | R     | 1207 | PRO  |
| 2   | M     | 340  | GLU  |
| 1   | R8    | 1207 | PRO  |
| 2   | M8    | 340  | GLU  |
| 1   | R16   | 1207 | PRO  |
| 2   | M16   | 340  | GLU  |
| 6   | O     | 278  | GLY  |
| 6   | O8    | 278  | GLY  |
| 6   | O16   | 278  | GLY  |
| 9   | K     | 725  | SER  |
| 9   | K8    | 725  | SER  |
| 9   | K16   | 1049 | ASP  |
| 10  | C16   | 620  | PRO  |
| 10  | C16   | 1066 | SER  |
| 10  | C16   | 1071 | GLN  |
| 10  | C24   | 620  | PRO  |
| 10  | C24   | 1066 | SER  |
| 10  | C24   | 1071 | GLN  |
| 14  | W     | 347  | ARG  |
| 14  | W     | 364  | SER  |
| 14  | W     | 600  | PRO  |
| 10  | C     | 620  | PRO  |
| 10  | C     | 1066 | SER  |
| 10  | C     | 1071 | GLN  |
| 10  | C8    | 620  | PRO  |
| 10  | C8    | 1066 | SER  |
| 10  | C8    | 1071 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B     | 607  | GLU  |
| 18  | B     | 678  | PRO  |
| 18  | B     | 694  | GLY  |
| 18  | B8    | 607  | GLU  |
| 18  | B8    | 678  | PRO  |
| 18  | B8    | 694  | GLY  |
| 19  | 4     | 186  | GLY  |
| 20  | E     | 339  | LYS  |
| 20  | E     | 352  | PHE  |
| 19  | 48    | 186  | GLY  |
| 20  | E8    | 339  | LYS  |
| 20  | E8    | 352  | PHE  |
| 24  | D     | 363  | PHE  |
| 24  | D     | 682  | THR  |
| 24  | D8    | 363  | PHE  |
| 24  | D8    | 682  | THR  |
| 24  | D16   | 363  | PHE  |
| 24  | D16   | 682  | THR  |
| 24  | D24   | 363  | PHE  |
| 24  | D24   | 682  | THR  |
| 24  | D32   | 363  | PHE  |
| 24  | D32   | 682  | THR  |
| 24  | D40   | 363  | PHE  |
| 24  | D40   | 682  | THR  |
| 10  | C32   | 620  | PRO  |
| 10  | C32   | 1066 | SER  |
| 10  | C32   | 1071 | GLN  |
| 1   | R8    | 215  | ASP  |
| 2   | M8    | 353  | ILE  |
| 1   | R16   | 215  | ASP  |
| 2   | M16   | 353  | ILE  |
| 13  | V     | 876  | PRO  |
| 10  | C     | 625  | SER  |
| 18  | B     | 855  | GLY  |
| 18  | B8    | 855  | GLY  |
| 24  | D     | 1200 | ASN  |
| 24  | D8    | 1200 | ASN  |
| 24  | D16   | 1200 | ASN  |
| 24  | D24   | 1200 | ASN  |
| 24  | D32   | 1200 | ASN  |
| 24  | D40   | 1200 | ASN  |
| 10  | C32   | 625  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 353  | ILE  |
| 3   | N     | 54   | GLY  |
| 3   | N8    | 54   | GLY  |
| 3   | N16   | 54   | GLY  |
| 14  | W     | 346  | VAL  |
| 18  | B     | 1064 | ILE  |
| 18  | B8    | 1064 | ILE  |
| 19  | 4     | 445  | VAL  |
| 20  | E     | 447  | ILE  |
| 19  | 48    | 445  | VAL  |
| 20  | E8    | 447  | ILE  |
| 5   | P     | 145  | ILE  |
| 5   | P8    | 145  | ILE  |
| 5   | P16   | 145  | ILE  |
| 13  | V     | 834  | PRO  |
| 17  | F     | 74   | ILE  |
| 17  | F24   | 74   | ILE  |
| 18  | B     | 989  | ILE  |
| 18  | B     | 1669 | PRO  |
| 18  | B8    | 989  | ILE  |
| 18  | B8    | 1669 | PRO  |
| 20  | E     | 344  | PRO  |
| 20  | E     | 347  | PRO  |
| 20  | E8    | 344  | PRO  |
| 20  | E8    | 347  | PRO  |
| 24  | D     | 61   | GLY  |
| 24  | D     | 402  | GLY  |
| 24  | D     | 1326 | ILE  |
| 24  | D8    | 61   | GLY  |
| 24  | D8    | 402  | GLY  |
| 24  | D8    | 1326 | ILE  |
| 24  | D16   | 61   | GLY  |
| 24  | D16   | 402  | GLY  |
| 24  | D16   | 1326 | ILE  |
| 24  | D24   | 61   | GLY  |
| 24  | D24   | 402  | GLY  |
| 24  | D24   | 1326 | ILE  |
| 24  | D32   | 61   | GLY  |
| 24  | D32   | 402  | GLY  |
| 24  | D32   | 1326 | ILE  |
| 24  | D40   | 61   | GLY  |
| 24  | D40   | 402  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D40   | 1326 | ILE  |
| 4   | T     | 319  | VAL  |
| 4   | T8    | 319  | VAL  |
| 4   | T16   | 319  | VAL  |
| 9   | K     | 978  | GLY  |
| 9   | K8    | 978  | GLY  |
| 10  | C16   | 1053 | GLY  |
| 11  | A24   | 512  | VAL  |
| 10  | C24   | 1053 | GLY  |
| 11  | A40   | 512  | VAL  |
| 12  | A     | 512  | VAL  |
| 10  | C     | 1053 | GLY  |
| 10  | C8    | 1053 | GLY  |
| 11  | A16   | 512  | VAL  |
| 17  | F8    | 74   | ILE  |
| 11  | A32   | 512  | VAL  |
| 17  | F16   | 74   | ILE  |
| 18  | B     | 1799 | VAL  |
| 18  | B8    | 1799 | VAL  |
| 20  | E     | 210  | VAL  |
| 20  | E8    | 210  | VAL  |
| 10  | C32   | 1053 | GLY  |
| 12  | A48   | 512  | VAL  |
| 14  | W     | 423  | VAL  |
| 18  | B     | 1115 | VAL  |
| 18  | B8    | 1115 | VAL  |
| 23  | J32   | 734  | PRO  |
| 23  | J8    | 734  | PRO  |
| 23  | J24   | 734  | PRO  |
| 23  | J16   | 734  | PRO  |
| 5   | P     | 589  | GLY  |
| 19  | 4     | 100  | ILE  |
| 19  | 48    | 100  | ILE  |
| 20  | E8    | 206  | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1   | R     | 1286/1314 (98%)  | 1245 (97%) | 41 (3%)   | 34          | 56 |
| 1   | R16   | 1286/1314 (98%)  | 1247 (97%) | 39 (3%)   | 36          | 57 |
| 1   | R8    | 1286/1314 (98%)  | 1246 (97%) | 40 (3%)   | 35          | 56 |
| 2   | M     | 619/626 (99%)    | 598 (97%)  | 21 (3%)   | 32          | 54 |
| 2   | M16   | 619/626 (99%)    | 599 (97%)  | 20 (3%)   | 34          | 56 |
| 2   | M8    | 619/626 (99%)    | 597 (96%)  | 22 (4%)   | 31          | 52 |
| 3   | N     | 246/246 (100%)   | 243 (99%)  | 3 (1%)    | 63          | 75 |
| 3   | N16   | 246/246 (100%)   | 242 (98%)  | 4 (2%)    | 55          | 70 |
| 3   | N8    | 246/246 (100%)   | 244 (99%)  | 2 (1%)    | 73          | 80 |
| 4   | T     | 611/611 (100%)   | 590 (97%)  | 21 (3%)   | 32          | 54 |
| 4   | T16   | 611/611 (100%)   | 596 (98%)  | 15 (2%)   | 42          | 63 |
| 4   | T8    | 611/611 (100%)   | 592 (97%)  | 19 (3%)   | 35          | 56 |
| 5   | P     | 622/629 (99%)    | 603 (97%)  | 19 (3%)   | 35          | 56 |
| 5   | P16   | 622/629 (99%)    | 606 (97%)  | 16 (3%)   | 40          | 62 |
| 5   | P8    | 622/629 (99%)    | 604 (97%)  | 18 (3%)   | 37          | 58 |
| 6   | O     | 262/280 (94%)    | 257 (98%)  | 5 (2%)    | 50          | 67 |
| 6   | O16   | 262/280 (94%)    | 257 (98%)  | 5 (2%)    | 50          | 67 |
| 6   | O8    | 262/280 (94%)    | 257 (98%)  | 5 (2%)    | 50          | 67 |
| 7   | Q     | 302/302 (100%)   | 297 (98%)  | 5 (2%)    | 53          | 69 |
| 7   | Q16   | 302/302 (100%)   | 298 (99%)  | 4 (1%)    | 61          | 74 |
| 7   | Q8    | 302/302 (100%)   | 299 (99%)  | 3 (1%)    | 68          | 78 |
| 8   | L     | 859/861 (100%)   | 853 (99%)  | 6 (1%)    | 76          | 81 |
| 8   | L16   | 859/861 (100%)   | 851 (99%)  | 8 (1%)    | 70          | 79 |
| 8   | L8    | 859/861 (100%)   | 853 (99%)  | 6 (1%)    | 76          | 81 |
| 9   | K     | 621/623 (100%)   | 569 (92%)  | 52 (8%)   | 10          | 30 |
| 9   | K16   | 621/623 (100%)   | 616 (99%)  | 5 (1%)    | 73          | 80 |
| 9   | K8    | 621/623 (100%)   | 570 (92%)  | 51 (8%)   | 10          | 31 |
| 10  | C     | 1628/1641 (99%)  | 1473 (90%) | 155 (10%) | 8           | 25 |
| 10  | C16   | 1641/1641 (100%) | 1488 (91%) | 153 (9%)  | 8           | 26 |
| 10  | C24   | 1641/1641 (100%) | 1498 (91%) | 143 (9%)  | 9           | 29 |
| 10  | C32   | 1641/1641 (100%) | 1499 (91%) | 142 (9%)  | 9           | 29 |
| 10  | C8    | 1598/1641 (97%)  | 1451 (91%) | 147 (9%)  | 8           | 27 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 11  | A16   | 696/730 (95%)    | 676 (97%)  | 20 (3%)  | 37          | 58 |
| 11  | A24   | 696/730 (95%)    | 678 (97%)  | 18 (3%)  | 40          | 62 |
| 11  | A32   | 696/730 (95%)    | 676 (97%)  | 20 (3%)  | 37          | 58 |
| 11  | A40   | 696/730 (95%)    | 678 (97%)  | 18 (3%)  | 40          | 62 |
| 12  | A     | 614/647 (95%)    | 597 (97%)  | 17 (3%)  | 38          | 60 |
| 12  | A48   | 617/647 (95%)    | 602 (98%)  | 15 (2%)  | 43          | 64 |
| 13  | V     | 175/175 (100%)   | 154 (88%)  | 21 (12%) | 5           | 17 |
| 14  | W     | 693/715 (97%)    | 665 (96%)  | 28 (4%)  | 28          | 49 |
| 15  | J     | 166/166 (100%)   | 156 (94%)  | 10 (6%)  | 17          | 39 |
| 16  | A8    | 59/59 (100%)     | 55 (93%)   | 4 (7%)   | 14          | 36 |
| 17  | F     | 25/25 (100%)     | 22 (88%)   | 3 (12%)  | 5           | 17 |
| 17  | F16   | 25/25 (100%)     | 22 (88%)   | 3 (12%)  | 5           | 17 |
| 17  | F24   | 25/25 (100%)     | 22 (88%)   | 3 (12%)  | 5           | 17 |
| 17  | F8    | 25/25 (100%)     | 22 (88%)   | 3 (12%)  | 5           | 17 |
| 18  | B     | 1759/1759 (100%) | 1652 (94%) | 107 (6%) | 17          | 38 |
| 18  | B8    | 1759/1759 (100%) | 1654 (94%) | 105 (6%) | 17          | 39 |
| 19  | 4     | 374/374 (100%)   | 356 (95%)  | 18 (5%)  | 23          | 44 |
| 19  | 48    | 374/374 (100%)   | 355 (95%)  | 19 (5%)  | 21          | 42 |
| 20  | E     | 450/450 (100%)   | 425 (94%)  | 25 (6%)  | 19          | 40 |
| 20  | E8    | 450/450 (100%)   | 423 (94%)  | 27 (6%)  | 17          | 39 |
| 21  | H     | 223/223 (100%)   | 217 (97%)  | 6 (3%)   | 39          | 61 |
| 21  | H16   | 223/223 (100%)   | 220 (99%)  | 3 (1%)   | 61          | 74 |
| 21  | H24   | 223/223 (100%)   | 220 (99%)  | 3 (1%)   | 61          | 74 |
| 21  | H8    | 223/223 (100%)   | 217 (97%)  | 6 (3%)   | 39          | 61 |
| 22  | I     | 212/212 (100%)   | 204 (96%)  | 8 (4%)   | 29          | 50 |
| 22  | I16   | 212/212 (100%)   | 202 (95%)  | 10 (5%)  | 23          | 45 |
| 22  | I24   | 212/212 (100%)   | 202 (95%)  | 10 (5%)  | 23          | 45 |
| 22  | I8    | 212/212 (100%)   | 203 (96%)  | 9 (4%)   | 26          | 48 |
| 23  | J16   | 176/176 (100%)   | 168 (96%)  | 8 (4%)   | 24          | 46 |
| 23  | J24   | 176/176 (100%)   | 168 (96%)  | 8 (4%)   | 24          | 46 |
| 23  | J32   | 176/176 (100%)   | 168 (96%)  | 8 (4%)   | 24          | 46 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers  | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|-------------|----|
| 23  | J8    | 176/176 (100%)    | 168 (96%)   | 8 (4%)    | 24          | 46 |
| 24  | D     | 1214/1223 (99%)   | 1201 (99%)  | 13 (1%)   | 65          | 76 |
| 24  | D16   | 1214/1223 (99%)   | 1197 (99%)  | 17 (1%)   | 59          | 72 |
| 24  | D24   | 1214/1223 (99%)   | 1196 (98%)  | 18 (2%)   | 57          | 72 |
| 24  | D32   | 1214/1223 (99%)   | 1197 (99%)  | 17 (1%)   | 59          | 72 |
| 24  | D40   | 1214/1223 (99%)   | 1197 (99%)  | 17 (1%)   | 59          | 72 |
| 24  | D8    | 1214/1223 (99%)   | 1201 (99%)  | 13 (1%)   | 65          | 76 |
| All | All   | 44535/45058 (99%) | 42674 (96%) | 1861 (4%) | 28          | 48 |

All (1861) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 43  | ASN  |
| 1   | R     | 69  | SER  |
| 1   | R     | 223 | THR  |
| 1   | R     | 359 | THR  |
| 1   | R     | 393 | SER  |
| 1   | R     | 395 | HIS  |
| 1   | R     | 396 | ASP  |
| 1   | R     | 440 | LEU  |
| 1   | R     | 448 | ASP  |
| 1   | R     | 466 | LEU  |
| 1   | R     | 481 | HIS  |
| 1   | R     | 499 | GLU  |
| 1   | R     | 522 | PHE  |
| 1   | R     | 538 | HIS  |
| 1   | R     | 541 | LEU  |
| 1   | R     | 548 | VAL  |
| 1   | R     | 554 | GLU  |
| 1   | R     | 563 | THR  |
| 1   | R     | 608 | THR  |
| 1   | R     | 613 | THR  |
| 1   | R     | 627 | LEU  |
| 1   | R     | 638 | ILE  |
| 1   | R     | 680 | GLU  |
| 1   | R     | 722 | VAL  |
| 1   | R     | 793 | PHE  |
| 1   | R     | 800 | LEU  |
| 1   | R     | 855 | LEU  |
| 1   | R     | 964 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R     | 1011 | THR  |
| 1   | R     | 1131 | MET  |
| 1   | R     | 1144 | CYS  |
| 1   | R     | 1185 | THR  |
| 1   | R     | 1186 | THR  |
| 1   | R     | 1188 | TYR  |
| 1   | R     | 1201 | LEU  |
| 1   | R     | 1244 | LEU  |
| 1   | R     | 1324 | ASP  |
| 1   | R     | 1329 | LEU  |
| 1   | R     | 1462 | GLU  |
| 1   | R     | 1475 | LEU  |
| 1   | R     | 1494 | THR  |
| 2   | M     | 164  | HIS  |
| 2   | M     | 206  | SER  |
| 2   | M     | 328  | THR  |
| 2   | M     | 331  | LEU  |
| 2   | M     | 332  | MET  |
| 2   | M     | 344  | GLN  |
| 2   | M     | 355  | THR  |
| 2   | M     | 448  | ASP  |
| 2   | M     | 505  | LEU  |
| 2   | M     | 507  | LEU  |
| 2   | M     | 755  | THR  |
| 2   | M     | 756  | MET  |
| 2   | M     | 759  | LEU  |
| 2   | M     | 762  | LEU  |
| 2   | M     | 764  | SER  |
| 2   | M     | 776  | LEU  |
| 2   | M     | 778  | GLU  |
| 2   | M     | 815  | SER  |
| 2   | M     | 846  | LEU  |
| 2   | M     | 849  | LEU  |
| 2   | M     | 854  | THR  |
| 3   | N     | 1    | MET  |
| 3   | N     | 167  | LEU  |
| 3   | N     | 170  | SER  |
| 1   | R8    | 55   | LEU  |
| 1   | R8    | 223  | THR  |
| 1   | R8    | 359  | THR  |
| 1   | R8    | 393  | SER  |
| 1   | R8    | 395  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R8    | 396  | ASP  |
| 1   | R8    | 440  | LEU  |
| 1   | R8    | 448  | ASP  |
| 1   | R8    | 466  | LEU  |
| 1   | R8    | 481  | HIS  |
| 1   | R8    | 499  | GLU  |
| 1   | R8    | 522  | PHE  |
| 1   | R8    | 538  | HIS  |
| 1   | R8    | 541  | LEU  |
| 1   | R8    | 548  | VAL  |
| 1   | R8    | 554  | GLU  |
| 1   | R8    | 563  | THR  |
| 1   | R8    | 608  | THR  |
| 1   | R8    | 613  | THR  |
| 1   | R8    | 627  | LEU  |
| 1   | R8    | 638  | ILE  |
| 1   | R8    | 680  | GLU  |
| 1   | R8    | 722  | VAL  |
| 1   | R8    | 793  | PHE  |
| 1   | R8    | 800  | LEU  |
| 1   | R8    | 855  | LEU  |
| 1   | R8    | 964  | THR  |
| 1   | R8    | 1011 | THR  |
| 1   | R8    | 1131 | MET  |
| 1   | R8    | 1144 | CYS  |
| 1   | R8    | 1185 | THR  |
| 1   | R8    | 1186 | THR  |
| 1   | R8    | 1188 | TYR  |
| 1   | R8    | 1201 | LEU  |
| 1   | R8    | 1244 | LEU  |
| 1   | R8    | 1324 | ASP  |
| 1   | R8    | 1329 | LEU  |
| 1   | R8    | 1462 | GLU  |
| 1   | R8    | 1475 | LEU  |
| 1   | R8    | 1494 | THR  |
| 2   | M8    | 164  | HIS  |
| 2   | M8    | 206  | SER  |
| 2   | M8    | 328  | THR  |
| 2   | M8    | 331  | LEU  |
| 2   | M8    | 332  | MET  |
| 2   | M8    | 344  | GLN  |
| 2   | M8    | 355  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M8    | 448 | ASP  |
| 2   | M8    | 505 | LEU  |
| 2   | M8    | 507 | LEU  |
| 2   | M8    | 627 | TYR  |
| 2   | M8    | 755 | THR  |
| 2   | M8    | 756 | MET  |
| 2   | M8    | 759 | LEU  |
| 2   | M8    | 762 | LEU  |
| 2   | M8    | 764 | SER  |
| 2   | M8    | 776 | LEU  |
| 2   | M8    | 778 | GLU  |
| 2   | M8    | 815 | SER  |
| 2   | M8    | 846 | LEU  |
| 2   | M8    | 849 | LEU  |
| 2   | M8    | 854 | THR  |
| 3   | N8    | 167 | LEU  |
| 3   | N8    | 170 | SER  |
| 1   | R16   | 43  | ASN  |
| 1   | R16   | 69  | SER  |
| 1   | R16   | 132 | LEU  |
| 1   | R16   | 223 | THR  |
| 1   | R16   | 359 | THR  |
| 1   | R16   | 393 | SER  |
| 1   | R16   | 395 | HIS  |
| 1   | R16   | 396 | ASP  |
| 1   | R16   | 440 | LEU  |
| 1   | R16   | 448 | ASP  |
| 1   | R16   | 466 | LEU  |
| 1   | R16   | 481 | HIS  |
| 1   | R16   | 522 | PHE  |
| 1   | R16   | 538 | HIS  |
| 1   | R16   | 541 | LEU  |
| 1   | R16   | 548 | VAL  |
| 1   | R16   | 554 | GLU  |
| 1   | R16   | 563 | THR  |
| 1   | R16   | 613 | THR  |
| 1   | R16   | 627 | LEU  |
| 1   | R16   | 677 | ASN  |
| 1   | R16   | 722 | VAL  |
| 1   | R16   | 793 | PHE  |
| 1   | R16   | 855 | LEU  |
| 1   | R16   | 964 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R16   | 1011 | THR  |
| 1   | R16   | 1131 | MET  |
| 1   | R16   | 1144 | CYS  |
| 1   | R16   | 1156 | GLU  |
| 1   | R16   | 1185 | THR  |
| 1   | R16   | 1186 | THR  |
| 1   | R16   | 1188 | TYR  |
| 1   | R16   | 1201 | LEU  |
| 1   | R16   | 1324 | ASP  |
| 1   | R16   | 1329 | LEU  |
| 1   | R16   | 1347 | HIS  |
| 1   | R16   | 1462 | GLU  |
| 1   | R16   | 1475 | LEU  |
| 1   | R16   | 1494 | THR  |
| 2   | M16   | 164  | HIS  |
| 2   | M16   | 206  | SER  |
| 2   | M16   | 328  | THR  |
| 2   | M16   | 332  | MET  |
| 2   | M16   | 355  | THR  |
| 2   | M16   | 448  | ASP  |
| 2   | M16   | 505  | LEU  |
| 2   | M16   | 507  | LEU  |
| 2   | M16   | 627  | TYR  |
| 2   | M16   | 755  | THR  |
| 2   | M16   | 756  | MET  |
| 2   | M16   | 759  | LEU  |
| 2   | M16   | 761  | PRO  |
| 2   | M16   | 764  | SER  |
| 2   | M16   | 776  | LEU  |
| 2   | M16   | 778  | GLU  |
| 2   | M16   | 815  | SER  |
| 2   | M16   | 846  | LEU  |
| 2   | M16   | 849  | LEU  |
| 2   | M16   | 854  | THR  |
| 3   | N16   | 1    | MET  |
| 3   | N16   | 7    | GLU  |
| 3   | N16   | 167  | LEU  |
| 3   | N16   | 170  | SER  |
| 4   | T     | 1    | MET  |
| 4   | T     | 2    | ASP  |
| 4   | T     | 20   | THR  |
| 4   | T     | 45   | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | T     | 56  | THR  |
| 4   | T     | 69  | VAL  |
| 4   | T     | 105 | LEU  |
| 4   | T     | 121 | HIS  |
| 4   | T     | 129 | ASP  |
| 4   | T     | 198 | THR  |
| 4   | T     | 199 | LEU  |
| 4   | T     | 268 | ILE  |
| 4   | T     | 312 | ASP  |
| 4   | T     | 418 | THR  |
| 4   | T     | 494 | VAL  |
| 4   | T     | 541 | LYS  |
| 4   | T     | 553 | THR  |
| 4   | T     | 582 | ASN  |
| 4   | T     | 647 | MET  |
| 4   | T     | 656 | TRP  |
| 4   | T     | 660 | LEU  |
| 4   | T8    | 20  | THR  |
| 4   | T8    | 45  | CYS  |
| 4   | T8    | 56  | THR  |
| 4   | T8    | 69  | VAL  |
| 4   | T8    | 105 | LEU  |
| 4   | T8    | 121 | HIS  |
| 4   | T8    | 129 | ASP  |
| 4   | T8    | 198 | THR  |
| 4   | T8    | 199 | LEU  |
| 4   | T8    | 268 | ILE  |
| 4   | T8    | 312 | ASP  |
| 4   | T8    | 418 | THR  |
| 4   | T8    | 494 | VAL  |
| 4   | T8    | 541 | LYS  |
| 4   | T8    | 553 | THR  |
| 4   | T8    | 582 | ASN  |
| 4   | T8    | 647 | MET  |
| 4   | T8    | 656 | TRP  |
| 4   | T8    | 660 | LEU  |
| 4   | T16   | 45  | CYS  |
| 4   | T16   | 56  | THR  |
| 4   | T16   | 105 | LEU  |
| 4   | T16   | 121 | HIS  |
| 4   | T16   | 129 | ASP  |
| 4   | T16   | 198 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | T16   | 268 | ILE  |
| 4   | T16   | 312 | ASP  |
| 4   | T16   | 418 | THR  |
| 4   | T16   | 541 | LYS  |
| 4   | T16   | 553 | THR  |
| 4   | T16   | 582 | ASN  |
| 4   | T16   | 647 | MET  |
| 4   | T16   | 656 | TRP  |
| 4   | T16   | 660 | LEU  |
| 5   | P     | 1   | MET  |
| 5   | P     | 8   | SER  |
| 5   | P     | 22  | THR  |
| 5   | P     | 25  | LEU  |
| 5   | P     | 62  | ASP  |
| 5   | P     | 144 | THR  |
| 5   | P     | 151 | LEU  |
| 5   | P     | 153 | GLU  |
| 5   | P     | 188 | LEU  |
| 5   | P     | 221 | LEU  |
| 5   | P     | 261 | LEU  |
| 5   | P     | 264 | LEU  |
| 5   | P     | 393 | VAL  |
| 5   | P     | 590 | SER  |
| 5   | P     | 598 | LEU  |
| 5   | P     | 611 | LEU  |
| 5   | P     | 620 | ILE  |
| 5   | P     | 678 | LEU  |
| 5   | P     | 689 | GLU  |
| 6   | O     | 29  | LEU  |
| 6   | O     | 38  | SER  |
| 6   | O     | 133 | LEU  |
| 6   | O     | 162 | THR  |
| 6   | O     | 163 | LEU  |
| 7   | Q     | 1   | MET  |
| 7   | Q     | 2   | GLU  |
| 7   | Q     | 29  | SER  |
| 7   | Q     | 221 | TRP  |
| 7   | Q     | 227 | SER  |
| 5   | P8    | 1   | MET  |
| 5   | P8    | 22  | THR  |
| 5   | P8    | 25  | LEU  |
| 5   | P8    | 62  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P8    | 144 | THR  |
| 5   | P8    | 151 | LEU  |
| 5   | P8    | 153 | GLU  |
| 5   | P8    | 188 | LEU  |
| 5   | P8    | 221 | LEU  |
| 5   | P8    | 261 | LEU  |
| 5   | P8    | 264 | LEU  |
| 5   | P8    | 393 | VAL  |
| 5   | P8    | 590 | SER  |
| 5   | P8    | 598 | LEU  |
| 5   | P8    | 611 | LEU  |
| 5   | P8    | 620 | ILE  |
| 5   | P8    | 678 | LEU  |
| 5   | P8    | 689 | GLU  |
| 6   | O8    | 29  | LEU  |
| 6   | O8    | 38  | SER  |
| 6   | O8    | 133 | LEU  |
| 6   | O8    | 162 | THR  |
| 6   | O8    | 163 | LEU  |
| 7   | Q8    | 29  | SER  |
| 7   | Q8    | 221 | TRP  |
| 7   | Q8    | 227 | SER  |
| 5   | P16   | 22  | THR  |
| 5   | P16   | 25  | LEU  |
| 5   | P16   | 62  | ASP  |
| 5   | P16   | 77  | SER  |
| 5   | P16   | 144 | THR  |
| 5   | P16   | 151 | LEU  |
| 5   | P16   | 221 | LEU  |
| 5   | P16   | 261 | LEU  |
| 5   | P16   | 264 | LEU  |
| 5   | P16   | 590 | SER  |
| 5   | P16   | 611 | LEU  |
| 5   | P16   | 620 | ILE  |
| 5   | P16   | 663 | LEU  |
| 5   | P16   | 678 | LEU  |
| 5   | P16   | 689 | GLU  |
| 5   | P16   | 712 | PHE  |
| 6   | O16   | 3   | LYS  |
| 6   | O16   | 29  | LEU  |
| 6   | O16   | 38  | SER  |
| 6   | O16   | 162 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | O16   | 163  | LEU  |
| 7   | Q16   | 29   | SER  |
| 7   | Q16   | 221  | TRP  |
| 7   | Q16   | 227  | SER  |
| 7   | Q16   | 335  | SER  |
| 8   | L     | 474  | THR  |
| 8   | L     | 553  | ASP  |
| 8   | L     | 655  | MET  |
| 8   | L     | 754  | VAL  |
| 8   | L     | 890  | THR  |
| 8   | L     | 968  | THR  |
| 8   | L8    | 474  | THR  |
| 8   | L8    | 553  | ASP  |
| 8   | L8    | 655  | MET  |
| 8   | L8    | 754  | VAL  |
| 8   | L8    | 890  | THR  |
| 8   | L8    | 968  | THR  |
| 8   | L16   | 264  | SER  |
| 8   | L16   | 474  | THR  |
| 8   | L16   | 553  | ASP  |
| 8   | L16   | 655  | MET  |
| 8   | L16   | 754  | VAL  |
| 8   | L16   | 890  | THR  |
| 8   | L16   | 968  | THR  |
| 8   | L16   | 1068 | PHE  |
| 9   | K     | 609  | SER  |
| 9   | K     | 629  | SER  |
| 9   | K     | 641  | THR  |
| 9   | K     | 703  | LEU  |
| 9   | K     | 709  | MET  |
| 9   | K     | 748  | THR  |
| 9   | K     | 752  | MET  |
| 9   | K     | 788  | LEU  |
| 9   | K     | 790  | THR  |
| 9   | K     | 831  | SER  |
| 9   | K     | 833  | THR  |
| 9   | K     | 842  | ILE  |
| 9   | K     | 847  | LEU  |
| 9   | K     | 850  | LEU  |
| 9   | K     | 857  | ASP  |
| 9   | K     | 883  | THR  |
| 9   | K     | 887  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | K     | 896  | LEU  |
| 9   | K     | 897  | LEU  |
| 9   | K     | 902  | THR  |
| 9   | K     | 910  | SER  |
| 9   | K     | 922  | GLU  |
| 9   | K     | 945  | LEU  |
| 9   | K     | 957  | ILE  |
| 9   | K     | 970  | LEU  |
| 9   | K     | 1005 | LEU  |
| 9   | K     | 1014 | LEU  |
| 9   | K     | 1026 | LEU  |
| 9   | K     | 1040 | THR  |
| 9   | K     | 1043 | THR  |
| 9   | K     | 1044 | LEU  |
| 9   | K     | 1060 | THR  |
| 9   | K     | 1104 | LEU  |
| 9   | K     | 1106 | LEU  |
| 9   | K     | 1107 | LEU  |
| 9   | K     | 1109 | LEU  |
| 9   | K     | 1114 | THR  |
| 9   | K     | 1117 | LEU  |
| 9   | K     | 1126 | LEU  |
| 9   | K     | 1132 | LEU  |
| 9   | K     | 1161 | GLU  |
| 9   | K     | 1166 | LEU  |
| 9   | K     | 1188 | THR  |
| 9   | K     | 1197 | THR  |
| 9   | K     | 1198 | LEU  |
| 9   | K     | 1199 | GLN  |
| 9   | K     | 1230 | LEU  |
| 9   | K     | 1232 | LEU  |
| 9   | K     | 1242 | SER  |
| 9   | K     | 1260 | LEU  |
| 9   | K     | 1263 | THR  |
| 9   | K     | 1269 | CYS  |
| 9   | K8    | 609  | SER  |
| 9   | K8    | 629  | SER  |
| 9   | K8    | 641  | THR  |
| 9   | K8    | 703  | LEU  |
| 9   | K8    | 709  | MET  |
| 9   | K8    | 748  | THR  |
| 9   | K8    | 752  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | K8    | 788  | LEU  |
| 9   | K8    | 790  | THR  |
| 9   | K8    | 831  | SER  |
| 9   | K8    | 833  | THR  |
| 9   | K8    | 842  | ILE  |
| 9   | K8    | 847  | LEU  |
| 9   | K8    | 850  | LEU  |
| 9   | K8    | 857  | ASP  |
| 9   | K8    | 883  | THR  |
| 9   | K8    | 887  | LEU  |
| 9   | K8    | 896  | LEU  |
| 9   | K8    | 897  | LEU  |
| 9   | K8    | 910  | SER  |
| 9   | K8    | 922  | GLU  |
| 9   | K8    | 945  | LEU  |
| 9   | K8    | 957  | ILE  |
| 9   | K8    | 970  | LEU  |
| 9   | K8    | 1005 | LEU  |
| 9   | K8    | 1014 | LEU  |
| 9   | K8    | 1026 | LEU  |
| 9   | K8    | 1040 | THR  |
| 9   | K8    | 1043 | THR  |
| 9   | K8    | 1044 | LEU  |
| 9   | K8    | 1060 | THR  |
| 9   | K8    | 1104 | LEU  |
| 9   | K8    | 1106 | LEU  |
| 9   | K8    | 1107 | LEU  |
| 9   | K8    | 1109 | LEU  |
| 9   | K8    | 1114 | THR  |
| 9   | K8    | 1117 | LEU  |
| 9   | K8    | 1126 | LEU  |
| 9   | K8    | 1132 | LEU  |
| 9   | K8    | 1161 | GLU  |
| 9   | K8    | 1166 | LEU  |
| 9   | K8    | 1188 | THR  |
| 9   | K8    | 1197 | THR  |
| 9   | K8    | 1198 | LEU  |
| 9   | K8    | 1199 | GLN  |
| 9   | K8    | 1230 | LEU  |
| 9   | K8    | 1232 | LEU  |
| 9   | K8    | 1242 | SER  |
| 9   | K8    | 1260 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | K8    | 1263 | THR  |
| 9   | K8    | 1269 | CYS  |
| 9   | K16   | 792  | LEU  |
| 9   | K16   | 930  | THR  |
| 9   | K16   | 1166 | LEU  |
| 9   | K16   | 1240 | SER  |
| 9   | K16   | 1281 | SER  |
| 10  | C16   | 14   | SER  |
| 10  | C16   | 22   | THR  |
| 10  | C16   | 24   | THR  |
| 10  | C16   | 28   | GLU  |
| 10  | C16   | 57   | VAL  |
| 10  | C16   | 58   | GLN  |
| 10  | C16   | 61   | GLU  |
| 10  | C16   | 65   | PRO  |
| 10  | C16   | 67   | SER  |
| 10  | C16   | 73   | ASP  |
| 10  | C16   | 74   | ASP  |
| 10  | C16   | 86   | GLU  |
| 10  | C16   | 89   | LEU  |
| 10  | C16   | 95   | VAL  |
| 10  | C16   | 105  | TRP  |
| 10  | C16   | 124  | TYR  |
| 10  | C16   | 156  | GLN  |
| 10  | C16   | 179  | ASN  |
| 10  | C16   | 180  | ARG  |
| 10  | C16   | 184  | THR  |
| 10  | C16   | 202  | LEU  |
| 10  | C16   | 248  | LEU  |
| 10  | C16   | 249  | THR  |
| 10  | C16   | 279  | LEU  |
| 10  | C16   | 280  | SER  |
| 10  | C16   | 284  | SER  |
| 10  | C16   | 294  | THR  |
| 10  | C16   | 303  | SER  |
| 10  | C16   | 308  | THR  |
| 10  | C16   | 313  | ILE  |
| 10  | C16   | 334  | MET  |
| 10  | C16   | 339  | THR  |
| 10  | C16   | 342  | THR  |
| 10  | C16   | 343  | THR  |
| 10  | C16   | 345  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C16   | 365 | LEU  |
| 10  | C16   | 379 | GLU  |
| 10  | C16   | 389 | LEU  |
| 10  | C16   | 415 | SER  |
| 10  | C16   | 422 | THR  |
| 10  | C16   | 423 | SER  |
| 10  | C16   | 424 | ASP  |
| 10  | C16   | 426 | LEU  |
| 10  | C16   | 427 | ASP  |
| 10  | C16   | 432 | THR  |
| 10  | C16   | 447 | PHE  |
| 10  | C16   | 450 | PRO  |
| 10  | C16   | 454 | SER  |
| 10  | C16   | 459 | LEU  |
| 10  | C16   | 461 | THR  |
| 10  | C16   | 485 | THR  |
| 10  | C16   | 499 | LEU  |
| 10  | C16   | 516 | CYS  |
| 10  | C16   | 528 | LEU  |
| 10  | C16   | 530 | THR  |
| 10  | C16   | 555 | LYS  |
| 10  | C16   | 563 | THR  |
| 10  | C16   | 572 | ILE  |
| 10  | C16   | 605 | GLU  |
| 10  | C16   | 619 | LEU  |
| 10  | C16   | 625 | SER  |
| 10  | C16   | 634 | SER  |
| 10  | C16   | 639 | MET  |
| 10  | C16   | 670 | GLU  |
| 10  | C16   | 672 | ASP  |
| 10  | C16   | 685 | CYS  |
| 10  | C16   | 703 | SER  |
| 10  | C16   | 716 | THR  |
| 10  | C16   | 721 | PHE  |
| 10  | C16   | 724 | SER  |
| 10  | C16   | 725 | LEU  |
| 10  | C16   | 727 | THR  |
| 10  | C16   | 728 | SER  |
| 10  | C16   | 730 | LEU  |
| 10  | C16   | 732 | THR  |
| 10  | C16   | 734 | LEU  |
| 10  | C16   | 749 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C16   | 753  | LEU  |
| 10  | C16   | 764  | ILE  |
| 10  | C16   | 798  | VAL  |
| 10  | C16   | 805  | LEU  |
| 10  | C16   | 814  | SER  |
| 10  | C16   | 827  | VAL  |
| 10  | C16   | 849  | SER  |
| 10  | C16   | 851  | LEU  |
| 10  | C16   | 866  | SER  |
| 10  | C16   | 879  | LEU  |
| 10  | C16   | 911  | ILE  |
| 10  | C16   | 984  | SER  |
| 10  | C16   | 994  | LEU  |
| 10  | C16   | 996  | THR  |
| 10  | C16   | 1006 | SER  |
| 10  | C16   | 1036 | SER  |
| 10  | C16   | 1041 | LEU  |
| 10  | C16   | 1049 | SER  |
| 10  | C16   | 1050 | HIS  |
| 10  | C16   | 1057 | THR  |
| 10  | C16   | 1068 | THR  |
| 10  | C16   | 1079 | THR  |
| 10  | C16   | 1081 | SER  |
| 10  | C16   | 1083 | SER  |
| 10  | C16   | 1085 | SER  |
| 10  | C16   | 1105 | LEU  |
| 10  | C16   | 1112 | LEU  |
| 10  | C16   | 1117 | LEU  |
| 10  | C16   | 1127 | THR  |
| 10  | C16   | 1132 | SER  |
| 10  | C16   | 1157 | LEU  |
| 10  | C16   | 1158 | HIS  |
| 10  | C16   | 1163 | LEU  |
| 10  | C16   | 1166 | SER  |
| 10  | C16   | 1173 | LEU  |
| 10  | C16   | 1208 | SER  |
| 10  | C16   | 1219 | ILE  |
| 10  | C16   | 1240 | SER  |
| 10  | C16   | 1275 | LEU  |
| 10  | C16   | 1277 | SER  |
| 10  | C16   | 1283 | LEU  |
| 10  | C16   | 1293 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C16   | 1309 | ARG  |
| 10  | C16   | 1341 | THR  |
| 10  | C16   | 1358 | ASP  |
| 10  | C16   | 1363 | ASP  |
| 10  | C16   | 1385 | LEU  |
| 10  | C16   | 1393 | SER  |
| 10  | C16   | 1445 | THR  |
| 10  | C16   | 1447 | LEU  |
| 10  | C16   | 1448 | LEU  |
| 10  | C16   | 1504 | ASP  |
| 10  | C16   | 1505 | MET  |
| 10  | C16   | 1507 | LEU  |
| 10  | C16   | 1538 | THR  |
| 10  | C16   | 1560 | GLN  |
| 10  | C16   | 1614 | LEU  |
| 10  | C16   | 1622 | SER  |
| 10  | C16   | 1624 | LEU  |
| 10  | C16   | 1628 | SER  |
| 10  | C16   | 1657 | SER  |
| 10  | C16   | 1658 | ASP  |
| 10  | C16   | 1661 | LEU  |
| 10  | C16   | 1665 | THR  |
| 10  | C16   | 1667 | LEU  |
| 10  | C16   | 1673 | LEU  |
| 10  | C16   | 1674 | LEU  |
| 10  | C16   | 1695 | LEU  |
| 10  | C16   | 1703 | ILE  |
| 10  | C16   | 1754 | LEU  |
| 10  | C16   | 1772 | ASP  |
| 10  | C16   | 1791 | GLN  |
| 10  | C16   | 1794 | THR  |
| 10  | C16   | 1827 | THR  |
| 10  | C16   | 1828 | THR  |
| 10  | C16   | 1832 | MET  |
| 11  | A24   | 27   | SER  |
| 11  | A24   | 52   | LEU  |
| 11  | A24   | 58   | SER  |
| 11  | A24   | 106  | GLN  |
| 11  | A24   | 156  | MET  |
| 11  | A24   | 160  | THR  |
| 11  | A24   | 242  | THR  |
| 11  | A24   | 309  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A24   | 333 | SER  |
| 11  | A24   | 334 | THR  |
| 11  | A24   | 438 | ARG  |
| 11  | A24   | 443 | LEU  |
| 11  | A24   | 466 | SER  |
| 11  | A24   | 467 | SER  |
| 11  | A24   | 524 | GLU  |
| 11  | A24   | 585 | MET  |
| 11  | A24   | 760 | LEU  |
| 11  | A24   | 835 | SER  |
| 10  | C24   | 8   | VAL  |
| 10  | C24   | 71  | SER  |
| 10  | C24   | 89  | LEU  |
| 10  | C24   | 98  | LEU  |
| 10  | C24   | 105 | TRP  |
| 10  | C24   | 124 | TYR  |
| 10  | C24   | 156 | GLN  |
| 10  | C24   | 179 | ASN  |
| 10  | C24   | 180 | ARG  |
| 10  | C24   | 184 | THR  |
| 10  | C24   | 202 | LEU  |
| 10  | C24   | 248 | LEU  |
| 10  | C24   | 249 | THR  |
| 10  | C24   | 279 | LEU  |
| 10  | C24   | 280 | SER  |
| 10  | C24   | 284 | SER  |
| 10  | C24   | 294 | THR  |
| 10  | C24   | 303 | SER  |
| 10  | C24   | 308 | THR  |
| 10  | C24   | 313 | ILE  |
| 10  | C24   | 334 | MET  |
| 10  | C24   | 339 | THR  |
| 10  | C24   | 342 | THR  |
| 10  | C24   | 343 | THR  |
| 10  | C24   | 345 | MET  |
| 10  | C24   | 365 | LEU  |
| 10  | C24   | 379 | GLU  |
| 10  | C24   | 389 | LEU  |
| 10  | C24   | 415 | SER  |
| 10  | C24   | 422 | THR  |
| 10  | C24   | 423 | SER  |
| 10  | C24   | 424 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C24   | 426 | LEU  |
| 10  | C24   | 427 | ASP  |
| 10  | C24   | 432 | THR  |
| 10  | C24   | 447 | PHE  |
| 10  | C24   | 450 | PRO  |
| 10  | C24   | 454 | SER  |
| 10  | C24   | 459 | LEU  |
| 10  | C24   | 461 | THR  |
| 10  | C24   | 485 | THR  |
| 10  | C24   | 499 | LEU  |
| 10  | C24   | 516 | CYS  |
| 10  | C24   | 528 | LEU  |
| 10  | C24   | 530 | THR  |
| 10  | C24   | 555 | LYS  |
| 10  | C24   | 563 | THR  |
| 10  | C24   | 572 | ILE  |
| 10  | C24   | 605 | GLU  |
| 10  | C24   | 619 | LEU  |
| 10  | C24   | 625 | SER  |
| 10  | C24   | 634 | SER  |
| 10  | C24   | 639 | MET  |
| 10  | C24   | 670 | GLU  |
| 10  | C24   | 672 | ASP  |
| 10  | C24   | 685 | CYS  |
| 10  | C24   | 703 | SER  |
| 10  | C24   | 716 | THR  |
| 10  | C24   | 721 | PHE  |
| 10  | C24   | 724 | SER  |
| 10  | C24   | 725 | LEU  |
| 10  | C24   | 727 | THR  |
| 10  | C24   | 728 | SER  |
| 10  | C24   | 730 | LEU  |
| 10  | C24   | 732 | THR  |
| 10  | C24   | 734 | LEU  |
| 10  | C24   | 749 | LEU  |
| 10  | C24   | 753 | LEU  |
| 10  | C24   | 764 | ILE  |
| 10  | C24   | 798 | VAL  |
| 10  | C24   | 805 | LEU  |
| 10  | C24   | 814 | SER  |
| 10  | C24   | 827 | VAL  |
| 10  | C24   | 849 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C24   | 851  | LEU  |
| 10  | C24   | 866  | SER  |
| 10  | C24   | 879  | LEU  |
| 10  | C24   | 911  | ILE  |
| 10  | C24   | 984  | SER  |
| 10  | C24   | 994  | LEU  |
| 10  | C24   | 996  | THR  |
| 10  | C24   | 1006 | SER  |
| 10  | C24   | 1036 | SER  |
| 10  | C24   | 1041 | LEU  |
| 10  | C24   | 1049 | SER  |
| 10  | C24   | 1050 | HIS  |
| 10  | C24   | 1057 | THR  |
| 10  | C24   | 1068 | THR  |
| 10  | C24   | 1079 | THR  |
| 10  | C24   | 1081 | SER  |
| 10  | C24   | 1083 | SER  |
| 10  | C24   | 1085 | SER  |
| 10  | C24   | 1105 | LEU  |
| 10  | C24   | 1112 | LEU  |
| 10  | C24   | 1117 | LEU  |
| 10  | C24   | 1127 | THR  |
| 10  | C24   | 1132 | SER  |
| 10  | C24   | 1157 | LEU  |
| 10  | C24   | 1158 | HIS  |
| 10  | C24   | 1163 | LEU  |
| 10  | C24   | 1166 | SER  |
| 10  | C24   | 1173 | LEU  |
| 10  | C24   | 1208 | SER  |
| 10  | C24   | 1219 | ILE  |
| 10  | C24   | 1240 | SER  |
| 10  | C24   | 1275 | LEU  |
| 10  | C24   | 1277 | SER  |
| 10  | C24   | 1283 | LEU  |
| 10  | C24   | 1293 | THR  |
| 10  | C24   | 1309 | ARG  |
| 10  | C24   | 1341 | THR  |
| 10  | C24   | 1358 | ASP  |
| 10  | C24   | 1363 | ASP  |
| 10  | C24   | 1385 | LEU  |
| 10  | C24   | 1393 | SER  |
| 10  | C24   | 1445 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C24   | 1447 | LEU  |
| 10  | C24   | 1448 | LEU  |
| 10  | C24   | 1504 | ASP  |
| 10  | C24   | 1505 | MET  |
| 10  | C24   | 1507 | LEU  |
| 10  | C24   | 1538 | THR  |
| 10  | C24   | 1560 | GLN  |
| 10  | C24   | 1614 | LEU  |
| 10  | C24   | 1622 | SER  |
| 10  | C24   | 1624 | LEU  |
| 10  | C24   | 1628 | SER  |
| 10  | C24   | 1657 | SER  |
| 10  | C24   | 1658 | ASP  |
| 10  | C24   | 1661 | LEU  |
| 10  | C24   | 1665 | THR  |
| 10  | C24   | 1667 | LEU  |
| 10  | C24   | 1673 | LEU  |
| 10  | C24   | 1674 | LEU  |
| 10  | C24   | 1695 | LEU  |
| 10  | C24   | 1703 | ILE  |
| 10  | C24   | 1754 | LEU  |
| 10  | C24   | 1772 | ASP  |
| 10  | C24   | 1791 | GLN  |
| 10  | C24   | 1794 | THR  |
| 10  | C24   | 1827 | THR  |
| 10  | C24   | 1828 | THR  |
| 10  | C24   | 1832 | MET  |
| 11  | A40   | 27   | SER  |
| 11  | A40   | 52   | LEU  |
| 11  | A40   | 58   | SER  |
| 11  | A40   | 106  | GLN  |
| 11  | A40   | 156  | MET  |
| 11  | A40   | 160  | THR  |
| 11  | A40   | 242  | THR  |
| 11  | A40   | 309  | VAL  |
| 11  | A40   | 333  | SER  |
| 11  | A40   | 334  | THR  |
| 11  | A40   | 438  | ARG  |
| 11  | A40   | 443  | LEU  |
| 11  | A40   | 466  | SER  |
| 11  | A40   | 467  | SER  |
| 11  | A40   | 524  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A40   | 585 | MET  |
| 11  | A40   | 760 | LEU  |
| 11  | A40   | 835 | SER  |
| 12  | A     | 102 | GLU  |
| 12  | A     | 106 | GLN  |
| 12  | A     | 156 | MET  |
| 12  | A     | 160 | THR  |
| 12  | A     | 242 | THR  |
| 12  | A     | 309 | VAL  |
| 12  | A     | 333 | SER  |
| 12  | A     | 334 | THR  |
| 12  | A     | 438 | ARG  |
| 12  | A     | 443 | LEU  |
| 12  | A     | 466 | SER  |
| 12  | A     | 467 | SER  |
| 12  | A     | 524 | GLU  |
| 12  | A     | 557 | LEU  |
| 12  | A     | 585 | MET  |
| 12  | A     | 760 | LEU  |
| 12  | A     | 835 | SER  |
| 13  | V     | 732 | SER  |
| 13  | V     | 743 | THR  |
| 13  | V     | 744 | LEU  |
| 13  | V     | 757 | SER  |
| 13  | V     | 762 | LEU  |
| 13  | V     | 782 | THR  |
| 13  | V     | 797 | LEU  |
| 13  | V     | 798 | LEU  |
| 13  | V     | 805 | LEU  |
| 13  | V     | 812 | GLU  |
| 13  | V     | 818 | THR  |
| 13  | V     | 826 | LEU  |
| 13  | V     | 832 | LEU  |
| 13  | V     | 846 | LEU  |
| 13  | V     | 854 | LEU  |
| 13  | V     | 882 | VAL  |
| 13  | V     | 889 | SER  |
| 13  | V     | 895 | LEU  |
| 13  | V     | 898 | LEU  |
| 13  | V     | 901 | THR  |
| 13  | V     | 921 | THR  |
| 14  | W     | 8   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | W     | 19  | THR  |
| 14  | W     | 38  | LEU  |
| 14  | W     | 306 | THR  |
| 14  | W     | 421 | LEU  |
| 14  | W     | 428 | LEU  |
| 14  | W     | 584 | CYS  |
| 14  | W     | 590 | LEU  |
| 14  | W     | 608 | SER  |
| 14  | W     | 609 | THR  |
| 14  | W     | 615 | GLU  |
| 14  | W     | 620 | LEU  |
| 14  | W     | 621 | LEU  |
| 14  | W     | 626 | LEU  |
| 14  | W     | 633 | GLU  |
| 14  | W     | 649 | LEU  |
| 14  | W     | 667 | ILE  |
| 14  | W     | 677 | LEU  |
| 14  | W     | 692 | GLU  |
| 14  | W     | 709 | LEU  |
| 14  | W     | 753 | THR  |
| 14  | W     | 768 | LEU  |
| 14  | W     | 777 | LEU  |
| 14  | W     | 781 | LEU  |
| 14  | W     | 784 | LEU  |
| 14  | W     | 787 | MET  |
| 14  | W     | 790 | ASP  |
| 14  | W     | 802 | LEU  |
| 15  | J     | 595 | THR  |
| 15  | J     | 605 | LEU  |
| 15  | J     | 617 | LEU  |
| 15  | J     | 635 | LEU  |
| 15  | J     | 648 | TYR  |
| 15  | J     | 687 | SER  |
| 15  | J     | 689 | LEU  |
| 15  | J     | 711 | GLU  |
| 15  | J     | 714 | SER  |
| 15  | J     | 722 | LEU  |
| 10  | C     | 8   | VAL  |
| 10  | C     | 28  | GLU  |
| 10  | C     | 39  | SER  |
| 10  | C     | 71  | SER  |
| 10  | C     | 89  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C     | 98  | LEU  |
| 10  | C     | 111 | ASP  |
| 10  | C     | 122 | LEU  |
| 10  | C     | 132 | SER  |
| 10  | C     | 158 | LEU  |
| 10  | C     | 169 | GLN  |
| 10  | C     | 173 | THR  |
| 10  | C     | 184 | THR  |
| 10  | C     | 195 | LEU  |
| 10  | C     | 202 | LEU  |
| 10  | C     | 248 | LEU  |
| 10  | C     | 249 | THR  |
| 10  | C     | 279 | LEU  |
| 10  | C     | 280 | SER  |
| 10  | C     | 284 | SER  |
| 10  | C     | 294 | THR  |
| 10  | C     | 303 | SER  |
| 10  | C     | 305 | SER  |
| 10  | C     | 308 | THR  |
| 10  | C     | 313 | ILE  |
| 10  | C     | 334 | MET  |
| 10  | C     | 339 | THR  |
| 10  | C     | 342 | THR  |
| 10  | C     | 343 | THR  |
| 10  | C     | 345 | MET  |
| 10  | C     | 365 | LEU  |
| 10  | C     | 389 | LEU  |
| 10  | C     | 415 | SER  |
| 10  | C     | 422 | THR  |
| 10  | C     | 423 | SER  |
| 10  | C     | 424 | ASP  |
| 10  | C     | 426 | LEU  |
| 10  | C     | 427 | ASP  |
| 10  | C     | 432 | THR  |
| 10  | C     | 454 | SER  |
| 10  | C     | 459 | LEU  |
| 10  | C     | 461 | THR  |
| 10  | C     | 485 | THR  |
| 10  | C     | 499 | LEU  |
| 10  | C     | 503 | THR  |
| 10  | C     | 516 | CYS  |
| 10  | C     | 528 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C     | 530 | THR  |
| 10  | C     | 535 | MET  |
| 10  | C     | 555 | LYS  |
| 10  | C     | 563 | THR  |
| 10  | C     | 572 | ILE  |
| 10  | C     | 605 | GLU  |
| 10  | C     | 619 | LEU  |
| 10  | C     | 625 | SER  |
| 10  | C     | 634 | SER  |
| 10  | C     | 639 | MET  |
| 10  | C     | 672 | ASP  |
| 10  | C     | 685 | CYS  |
| 10  | C     | 696 | GLN  |
| 10  | C     | 703 | SER  |
| 10  | C     | 709 | GLU  |
| 10  | C     | 716 | THR  |
| 10  | C     | 718 | HIS  |
| 10  | C     | 724 | SER  |
| 10  | C     | 725 | LEU  |
| 10  | C     | 727 | THR  |
| 10  | C     | 728 | SER  |
| 10  | C     | 730 | LEU  |
| 10  | C     | 732 | THR  |
| 10  | C     | 734 | LEU  |
| 10  | C     | 749 | LEU  |
| 10  | C     | 753 | LEU  |
| 10  | C     | 754 | MET  |
| 10  | C     | 764 | ILE  |
| 10  | C     | 798 | VAL  |
| 10  | C     | 805 | LEU  |
| 10  | C     | 812 | ILE  |
| 10  | C     | 814 | SER  |
| 10  | C     | 827 | VAL  |
| 10  | C     | 849 | SER  |
| 10  | C     | 851 | LEU  |
| 10  | C     | 866 | SER  |
| 10  | C     | 867 | LEU  |
| 10  | C     | 879 | LEU  |
| 10  | C     | 911 | ILE  |
| 10  | C     | 984 | SER  |
| 10  | C     | 994 | LEU  |
| 10  | C     | 996 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C     | 1002 | LEU  |
| 10  | C     | 1006 | SER  |
| 10  | C     | 1036 | SER  |
| 10  | C     | 1041 | LEU  |
| 10  | C     | 1049 | SER  |
| 10  | C     | 1050 | HIS  |
| 10  | C     | 1057 | THR  |
| 10  | C     | 1068 | THR  |
| 10  | C     | 1079 | THR  |
| 10  | C     | 1081 | SER  |
| 10  | C     | 1083 | SER  |
| 10  | C     | 1105 | LEU  |
| 10  | C     | 1112 | LEU  |
| 10  | C     | 1117 | LEU  |
| 10  | C     | 1127 | THR  |
| 10  | C     | 1132 | SER  |
| 10  | C     | 1157 | LEU  |
| 10  | C     | 1158 | HIS  |
| 10  | C     | 1163 | LEU  |
| 10  | C     | 1166 | SER  |
| 10  | C     | 1173 | LEU  |
| 10  | C     | 1178 | GLU  |
| 10  | C     | 1208 | SER  |
| 10  | C     | 1219 | ILE  |
| 10  | C     | 1240 | SER  |
| 10  | C     | 1247 | LEU  |
| 10  | C     | 1275 | LEU  |
| 10  | C     | 1277 | SER  |
| 10  | C     | 1283 | LEU  |
| 10  | C     | 1293 | THR  |
| 10  | C     | 1309 | ARG  |
| 10  | C     | 1341 | THR  |
| 10  | C     | 1363 | ASP  |
| 10  | C     | 1385 | LEU  |
| 10  | C     | 1387 | LEU  |
| 10  | C     | 1393 | SER  |
| 10  | C     | 1445 | THR  |
| 10  | C     | 1447 | LEU  |
| 10  | C     | 1448 | LEU  |
| 10  | C     | 1485 | LEU  |
| 10  | C     | 1504 | ASP  |
| 10  | C     | 1505 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C     | 1507 | LEU  |
| 10  | C     | 1560 | GLN  |
| 10  | C     | 1614 | LEU  |
| 10  | C     | 1622 | SER  |
| 10  | C     | 1624 | LEU  |
| 10  | C     | 1628 | SER  |
| 10  | C     | 1657 | SER  |
| 10  | C     | 1658 | ASP  |
| 10  | C     | 1661 | LEU  |
| 10  | C     | 1665 | THR  |
| 10  | C     | 1667 | LEU  |
| 10  | C     | 1673 | LEU  |
| 10  | C     | 1674 | LEU  |
| 10  | C     | 1686 | LEU  |
| 10  | C     | 1695 | LEU  |
| 10  | C     | 1703 | ILE  |
| 10  | C     | 1754 | LEU  |
| 10  | C     | 1772 | ASP  |
| 10  | C     | 1790 | GLN  |
| 10  | C     | 1791 | GLN  |
| 10  | C     | 1794 | THR  |
| 10  | C     | 1827 | THR  |
| 10  | C     | 1828 | THR  |
| 10  | C     | 1832 | MET  |
| 10  | C8    | 12   | HIS  |
| 10  | C8    | 14   | SER  |
| 10  | C8    | 27   | ILE  |
| 10  | C8    | 49   | PRO  |
| 10  | C8    | 51   | PRO  |
| 10  | C8    | 66   | ASP  |
| 10  | C8    | 67   | SER  |
| 10  | C8    | 79   | ILE  |
| 10  | C8    | 111  | ASP  |
| 10  | C8    | 122  | LEU  |
| 10  | C8    | 132  | SER  |
| 10  | C8    | 158  | LEU  |
| 10  | C8    | 169  | GLN  |
| 10  | C8    | 173  | THR  |
| 10  | C8    | 184  | THR  |
| 10  | C8    | 195  | LEU  |
| 10  | C8    | 202  | LEU  |
| 10  | C8    | 248  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C8    | 249 | THR  |
| 10  | C8    | 279 | LEU  |
| 10  | C8    | 280 | SER  |
| 10  | C8    | 284 | SER  |
| 10  | C8    | 294 | THR  |
| 10  | C8    | 303 | SER  |
| 10  | C8    | 305 | SER  |
| 10  | C8    | 308 | THR  |
| 10  | C8    | 313 | ILE  |
| 10  | C8    | 334 | MET  |
| 10  | C8    | 339 | THR  |
| 10  | C8    | 342 | THR  |
| 10  | C8    | 343 | THR  |
| 10  | C8    | 345 | MET  |
| 10  | C8    | 365 | LEU  |
| 10  | C8    | 389 | LEU  |
| 10  | C8    | 415 | SER  |
| 10  | C8    | 422 | THR  |
| 10  | C8    | 423 | SER  |
| 10  | C8    | 424 | ASP  |
| 10  | C8    | 426 | LEU  |
| 10  | C8    | 427 | ASP  |
| 10  | C8    | 432 | THR  |
| 10  | C8    | 454 | SER  |
| 10  | C8    | 459 | LEU  |
| 10  | C8    | 461 | THR  |
| 10  | C8    | 485 | THR  |
| 10  | C8    | 499 | LEU  |
| 10  | C8    | 503 | THR  |
| 10  | C8    | 516 | CYS  |
| 10  | C8    | 528 | LEU  |
| 10  | C8    | 530 | THR  |
| 10  | C8    | 535 | MET  |
| 10  | C8    | 555 | LYS  |
| 10  | C8    | 563 | THR  |
| 10  | C8    | 572 | ILE  |
| 10  | C8    | 605 | GLU  |
| 10  | C8    | 619 | LEU  |
| 10  | C8    | 639 | MET  |
| 10  | C8    | 672 | ASP  |
| 10  | C8    | 685 | CYS  |
| 10  | C8    | 696 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 703  | SER  |
| 10  | C8    | 709  | GLU  |
| 10  | C8    | 730  | LEU  |
| 10  | C8    | 732  | THR  |
| 10  | C8    | 734  | LEU  |
| 10  | C8    | 749  | LEU  |
| 10  | C8    | 753  | LEU  |
| 10  | C8    | 754  | MET  |
| 10  | C8    | 764  | ILE  |
| 10  | C8    | 798  | VAL  |
| 10  | C8    | 805  | LEU  |
| 10  | C8    | 812  | ILE  |
| 10  | C8    | 814  | SER  |
| 10  | C8    | 827  | VAL  |
| 10  | C8    | 849  | SER  |
| 10  | C8    | 851  | LEU  |
| 10  | C8    | 866  | SER  |
| 10  | C8    | 867  | LEU  |
| 10  | C8    | 879  | LEU  |
| 10  | C8    | 911  | ILE  |
| 10  | C8    | 984  | SER  |
| 10  | C8    | 994  | LEU  |
| 10  | C8    | 996  | THR  |
| 10  | C8    | 1002 | LEU  |
| 10  | C8    | 1006 | SER  |
| 10  | C8    | 1036 | SER  |
| 10  | C8    | 1041 | LEU  |
| 10  | C8    | 1049 | SER  |
| 10  | C8    | 1050 | HIS  |
| 10  | C8    | 1057 | THR  |
| 10  | C8    | 1068 | THR  |
| 10  | C8    | 1079 | THR  |
| 10  | C8    | 1081 | SER  |
| 10  | C8    | 1083 | SER  |
| 10  | C8    | 1105 | LEU  |
| 10  | C8    | 1112 | LEU  |
| 10  | C8    | 1117 | LEU  |
| 10  | C8    | 1127 | THR  |
| 10  | C8    | 1132 | SER  |
| 10  | C8    | 1157 | LEU  |
| 10  | C8    | 1158 | HIS  |
| 10  | C8    | 1163 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 1166 | SER  |
| 10  | C8    | 1173 | LEU  |
| 10  | C8    | 1178 | GLU  |
| 10  | C8    | 1208 | SER  |
| 10  | C8    | 1219 | ILE  |
| 10  | C8    | 1240 | SER  |
| 10  | C8    | 1247 | LEU  |
| 10  | C8    | 1275 | LEU  |
| 10  | C8    | 1277 | SER  |
| 10  | C8    | 1283 | LEU  |
| 10  | C8    | 1293 | THR  |
| 10  | C8    | 1309 | ARG  |
| 10  | C8    | 1341 | THR  |
| 10  | C8    | 1363 | ASP  |
| 10  | C8    | 1385 | LEU  |
| 10  | C8    | 1387 | LEU  |
| 10  | C8    | 1393 | SER  |
| 10  | C8    | 1445 | THR  |
| 10  | C8    | 1447 | LEU  |
| 10  | C8    | 1448 | LEU  |
| 10  | C8    | 1485 | LEU  |
| 10  | C8    | 1504 | ASP  |
| 10  | C8    | 1505 | MET  |
| 10  | C8    | 1507 | LEU  |
| 10  | C8    | 1538 | THR  |
| 10  | C8    | 1560 | GLN  |
| 10  | C8    | 1614 | LEU  |
| 10  | C8    | 1622 | SER  |
| 10  | C8    | 1624 | LEU  |
| 10  | C8    | 1628 | SER  |
| 10  | C8    | 1657 | SER  |
| 10  | C8    | 1673 | LEU  |
| 10  | C8    | 1674 | LEU  |
| 10  | C8    | 1686 | LEU  |
| 10  | C8    | 1695 | LEU  |
| 10  | C8    | 1703 | ILE  |
| 10  | C8    | 1754 | LEU  |
| 10  | C8    | 1772 | ASP  |
| 10  | C8    | 1790 | GLN  |
| 10  | C8    | 1791 | GLN  |
| 10  | C8    | 1794 | THR  |
| 10  | C8    | 1800 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 1827 | THR  |
| 10  | C8    | 1828 | THR  |
| 10  | C8    | 1832 | MET  |
| 16  | A8    | 102  | GLU  |
| 16  | A8    | 106  | GLN  |
| 16  | A8    | 156  | MET  |
| 16  | A8    | 160  | THR  |
| 11  | A16   | 27   | SER  |
| 11  | A16   | 52   | LEU  |
| 11  | A16   | 58   | SER  |
| 11  | A16   | 102  | GLU  |
| 11  | A16   | 111  | MET  |
| 11  | A16   | 115  | SER  |
| 11  | A16   | 158  | PRO  |
| 11  | A16   | 160  | THR  |
| 11  | A16   | 242  | THR  |
| 11  | A16   | 309  | VAL  |
| 11  | A16   | 333  | SER  |
| 11  | A16   | 334  | THR  |
| 11  | A16   | 438  | ARG  |
| 11  | A16   | 443  | LEU  |
| 11  | A16   | 466  | SER  |
| 11  | A16   | 467  | SER  |
| 11  | A16   | 524  | GLU  |
| 11  | A16   | 585  | MET  |
| 11  | A16   | 760  | LEU  |
| 11  | A16   | 835  | SER  |
| 17  | F8    | 72   | SER  |
| 17  | F8    | 78   | SER  |
| 17  | F8    | 80   | SER  |
| 17  | F     | 72   | SER  |
| 17  | F     | 78   | SER  |
| 17  | F     | 80   | SER  |
| 11  | A32   | 27   | SER  |
| 11  | A32   | 52   | LEU  |
| 11  | A32   | 58   | SER  |
| 11  | A32   | 102  | GLU  |
| 11  | A32   | 111  | MET  |
| 11  | A32   | 115  | SER  |
| 11  | A32   | 158  | PRO  |
| 11  | A32   | 160  | THR  |
| 11  | A32   | 242  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A32   | 309 | VAL  |
| 11  | A32   | 333 | SER  |
| 11  | A32   | 334 | THR  |
| 11  | A32   | 438 | ARG  |
| 11  | A32   | 443 | LEU  |
| 11  | A32   | 466 | SER  |
| 11  | A32   | 467 | SER  |
| 11  | A32   | 524 | GLU  |
| 11  | A32   | 585 | MET  |
| 11  | A32   | 760 | LEU  |
| 11  | A32   | 835 | SER  |
| 17  | F24   | 72  | SER  |
| 17  | F24   | 78  | SER  |
| 17  | F24   | 80  | SER  |
| 17  | F16   | 72  | SER  |
| 17  | F16   | 78  | SER  |
| 17  | F16   | 80  | SER  |
| 18  | B     | 32  | LEU  |
| 18  | B     | 58  | SER  |
| 18  | B     | 69  | LEU  |
| 18  | B     | 77  | LEU  |
| 18  | B     | 104 | LEU  |
| 18  | B     | 112 | GLU  |
| 18  | B     | 115 | THR  |
| 18  | B     | 116 | THR  |
| 18  | B     | 123 | LEU  |
| 18  | B     | 124 | THR  |
| 18  | B     | 134 | GLN  |
| 18  | B     | 188 | SER  |
| 18  | B     | 191 | PHE  |
| 18  | B     | 199 | LEU  |
| 18  | B     | 256 | VAL  |
| 18  | B     | 271 | LEU  |
| 18  | B     | 303 | ILE  |
| 18  | B     | 347 | SER  |
| 18  | B     | 353 | ILE  |
| 18  | B     | 380 | LEU  |
| 18  | B     | 411 | LEU  |
| 18  | B     | 491 | VAL  |
| 18  | B     | 509 | SER  |
| 18  | B     | 511 | LEU  |
| 18  | B     | 515 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B     | 518  | LEU  |
| 18  | B     | 526  | LEU  |
| 18  | B     | 541  | SER  |
| 18  | B     | 553  | LEU  |
| 18  | B     | 602  | PHE  |
| 18  | B     | 614  | MET  |
| 18  | B     | 671  | MET  |
| 18  | B     | 686  | LEU  |
| 18  | B     | 691  | SER  |
| 18  | B     | 748  | SER  |
| 18  | B     | 756  | HIS  |
| 18  | B     | 789  | LEU  |
| 18  | B     | 818  | SER  |
| 18  | B     | 856  | LEU  |
| 18  | B     | 982  | SER  |
| 18  | B     | 994  | CYS  |
| 18  | B     | 998  | LEU  |
| 18  | B     | 999  | LEU  |
| 18  | B     | 1010 | THR  |
| 18  | B     | 1021 | LEU  |
| 18  | B     | 1068 | THR  |
| 18  | B     | 1114 | CYS  |
| 18  | B     | 1120 | THR  |
| 18  | B     | 1130 | LEU  |
| 18  | B     | 1131 | THR  |
| 18  | B     | 1133 | THR  |
| 18  | B     | 1136 | SER  |
| 18  | B     | 1160 | SER  |
| 18  | B     | 1161 | LEU  |
| 18  | B     | 1186 | LEU  |
| 18  | B     | 1208 | THR  |
| 18  | B     | 1209 | LEU  |
| 18  | B     | 1219 | LEU  |
| 18  | B     | 1233 | LEU  |
| 18  | B     | 1249 | LEU  |
| 18  | B     | 1256 | THR  |
| 18  | B     | 1264 | GLN  |
| 18  | B     | 1285 | MET  |
| 18  | B     | 1287 | LEU  |
| 18  | B     | 1333 | LEU  |
| 18  | B     | 1392 | SER  |
| 18  | B     | 1422 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B     | 1438 | LEU  |
| 18  | B     | 1446 | HIS  |
| 18  | B     | 1447 | SER  |
| 18  | B     | 1462 | LEU  |
| 18  | B     | 1481 | MET  |
| 18  | B     | 1497 | LEU  |
| 18  | B     | 1498 | LEU  |
| 18  | B     | 1520 | LEU  |
| 18  | B     | 1530 | THR  |
| 18  | B     | 1548 | LEU  |
| 18  | B     | 1553 | SER  |
| 18  | B     | 1591 | MET  |
| 18  | B     | 1597 | MET  |
| 18  | B     | 1598 | SER  |
| 18  | B     | 1599 | THR  |
| 18  | B     | 1600 | LEU  |
| 18  | B     | 1602 | SER  |
| 18  | B     | 1609 | LEU  |
| 18  | B     | 1610 | LEU  |
| 18  | B     | 1613 | THR  |
| 18  | B     | 1678 | LEU  |
| 18  | B     | 1683 | THR  |
| 18  | B     | 1684 | TRP  |
| 18  | B     | 1685 | THR  |
| 18  | B     | 1700 | LEU  |
| 18  | B     | 1739 | LEU  |
| 18  | B     | 1749 | LEU  |
| 18  | B     | 1761 | SER  |
| 18  | B     | 1770 | THR  |
| 18  | B     | 1789 | THR  |
| 18  | B     | 1792 | SER  |
| 18  | B     | 1794 | SER  |
| 18  | B     | 1795 | THR  |
| 18  | B     | 1804 | THR  |
| 18  | B     | 1809 | SER  |
| 18  | B     | 1843 | THR  |
| 18  | B     | 1868 | LEU  |
| 18  | B     | 1959 | PHE  |
| 18  | B     | 1960 | LEU  |
| 18  | B     | 1965 | LEU  |
| 18  | B8    | 18   | SER  |
| 18  | B8    | 56   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B8    | 104  | LEU  |
| 18  | B8    | 112  | GLU  |
| 18  | B8    | 115  | THR  |
| 18  | B8    | 116  | THR  |
| 18  | B8    | 123  | LEU  |
| 18  | B8    | 124  | THR  |
| 18  | B8    | 134  | GLN  |
| 18  | B8    | 188  | SER  |
| 18  | B8    | 191  | PHE  |
| 18  | B8    | 199  | LEU  |
| 18  | B8    | 256  | VAL  |
| 18  | B8    | 271  | LEU  |
| 18  | B8    | 303  | ILE  |
| 18  | B8    | 347  | SER  |
| 18  | B8    | 353  | ILE  |
| 18  | B8    | 380  | LEU  |
| 18  | B8    | 411  | LEU  |
| 18  | B8    | 491  | VAL  |
| 18  | B8    | 509  | SER  |
| 18  | B8    | 511  | LEU  |
| 18  | B8    | 515  | SER  |
| 18  | B8    | 518  | LEU  |
| 18  | B8    | 526  | LEU  |
| 18  | B8    | 541  | SER  |
| 18  | B8    | 553  | LEU  |
| 18  | B8    | 602  | PHE  |
| 18  | B8    | 614  | MET  |
| 18  | B8    | 671  | MET  |
| 18  | B8    | 686  | LEU  |
| 18  | B8    | 691  | SER  |
| 18  | B8    | 748  | SER  |
| 18  | B8    | 756  | HIS  |
| 18  | B8    | 789  | LEU  |
| 18  | B8    | 818  | SER  |
| 18  | B8    | 856  | LEU  |
| 18  | B8    | 982  | SER  |
| 18  | B8    | 994  | CYS  |
| 18  | B8    | 998  | LEU  |
| 18  | B8    | 999  | LEU  |
| 18  | B8    | 1010 | THR  |
| 18  | B8    | 1021 | LEU  |
| 18  | B8    | 1068 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B8    | 1114 | CYS  |
| 18  | B8    | 1120 | THR  |
| 18  | B8    | 1130 | LEU  |
| 18  | B8    | 1131 | THR  |
| 18  | B8    | 1133 | THR  |
| 18  | B8    | 1136 | SER  |
| 18  | B8    | 1160 | SER  |
| 18  | B8    | 1161 | LEU  |
| 18  | B8    | 1186 | LEU  |
| 18  | B8    | 1208 | THR  |
| 18  | B8    | 1209 | LEU  |
| 18  | B8    | 1219 | LEU  |
| 18  | B8    | 1233 | LEU  |
| 18  | B8    | 1249 | LEU  |
| 18  | B8    | 1256 | THR  |
| 18  | B8    | 1264 | GLN  |
| 18  | B8    | 1285 | MET  |
| 18  | B8    | 1287 | LEU  |
| 18  | B8    | 1333 | LEU  |
| 18  | B8    | 1392 | SER  |
| 18  | B8    | 1422 | LEU  |
| 18  | B8    | 1438 | LEU  |
| 18  | B8    | 1446 | HIS  |
| 18  | B8    | 1447 | SER  |
| 18  | B8    | 1462 | LEU  |
| 18  | B8    | 1481 | MET  |
| 18  | B8    | 1497 | LEU  |
| 18  | B8    | 1498 | LEU  |
| 18  | B8    | 1520 | LEU  |
| 18  | B8    | 1530 | THR  |
| 18  | B8    | 1548 | LEU  |
| 18  | B8    | 1553 | SER  |
| 18  | B8    | 1591 | MET  |
| 18  | B8    | 1597 | MET  |
| 18  | B8    | 1598 | SER  |
| 18  | B8    | 1599 | THR  |
| 18  | B8    | 1600 | LEU  |
| 18  | B8    | 1602 | SER  |
| 18  | B8    | 1609 | LEU  |
| 18  | B8    | 1610 | LEU  |
| 18  | B8    | 1613 | THR  |
| 18  | B8    | 1678 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B8    | 1683 | THR  |
| 18  | B8    | 1684 | TRP  |
| 18  | B8    | 1685 | THR  |
| 18  | B8    | 1700 | LEU  |
| 18  | B8    | 1739 | LEU  |
| 18  | B8    | 1749 | LEU  |
| 18  | B8    | 1761 | SER  |
| 18  | B8    | 1770 | THR  |
| 18  | B8    | 1789 | THR  |
| 18  | B8    | 1792 | SER  |
| 18  | B8    | 1794 | SER  |
| 18  | B8    | 1795 | THR  |
| 18  | B8    | 1804 | THR  |
| 18  | B8    | 1809 | SER  |
| 18  | B8    | 1843 | THR  |
| 18  | B8    | 1868 | LEU  |
| 18  | B8    | 1959 | PHE  |
| 18  | B8    | 1960 | LEU  |
| 18  | B8    | 1965 | LEU  |
| 19  | 4     | 33   | THR  |
| 19  | 4     | 40   | MET  |
| 19  | 4     | 50   | THR  |
| 19  | 4     | 70   | SER  |
| 19  | 4     | 73   | LEU  |
| 19  | 4     | 76   | THR  |
| 19  | 4     | 77   | LEU  |
| 19  | 4     | 85   | LEU  |
| 19  | 4     | 92   | THR  |
| 19  | 4     | 95   | THR  |
| 19  | 4     | 101  | ASP  |
| 19  | 4     | 164  | CYS  |
| 19  | 4     | 189  | LEU  |
| 19  | 4     | 192  | SER  |
| 19  | 4     | 193  | LEU  |
| 19  | 4     | 306  | ASP  |
| 19  | 4     | 313  | LEU  |
| 19  | 4     | 412  | SER  |
| 20  | E     | 39   | SER  |
| 20  | E     | 51   | LEU  |
| 20  | E     | 79   | LEU  |
| 20  | E     | 85   | LEU  |
| 20  | E     | 89   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | E     | 124 | LEU  |
| 20  | E     | 196 | MET  |
| 20  | E     | 197 | LEU  |
| 20  | E     | 201 | LEU  |
| 20  | E     | 202 | ASP  |
| 20  | E     | 203 | TRP  |
| 20  | E     | 207 | LEU  |
| 20  | E     | 209 | SER  |
| 20  | E     | 214 | LEU  |
| 20  | E     | 219 | LEU  |
| 20  | E     | 308 | GLU  |
| 20  | E     | 337 | THR  |
| 20  | E     | 343 | THR  |
| 20  | E     | 345 | LEU  |
| 20  | E     | 349 | THR  |
| 20  | E     | 426 | LEU  |
| 20  | E     | 436 | THR  |
| 20  | E     | 437 | SER  |
| 20  | E     | 454 | MET  |
| 20  | E     | 494 | ILE  |
| 19  | 48    | 5   | PRO  |
| 19  | 48    | 33  | THR  |
| 19  | 48    | 40  | MET  |
| 19  | 48    | 50  | THR  |
| 19  | 48    | 70  | SER  |
| 19  | 48    | 73  | LEU  |
| 19  | 48    | 76  | THR  |
| 19  | 48    | 77  | LEU  |
| 19  | 48    | 85  | LEU  |
| 19  | 48    | 92  | THR  |
| 19  | 48    | 95  | THR  |
| 19  | 48    | 101 | ASP  |
| 19  | 48    | 164 | CYS  |
| 19  | 48    | 189 | LEU  |
| 19  | 48    | 192 | SER  |
| 19  | 48    | 193 | LEU  |
| 19  | 48    | 306 | ASP  |
| 19  | 48    | 313 | LEU  |
| 19  | 48    | 412 | SER  |
| 20  | E8    | 5   | PRO  |
| 20  | E8    | 9   | THR  |
| 20  | E8    | 39  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | E8    | 51  | LEU  |
| 20  | E8    | 79  | LEU  |
| 20  | E8    | 85  | LEU  |
| 20  | E8    | 89  | LEU  |
| 20  | E8    | 124 | LEU  |
| 20  | E8    | 196 | MET  |
| 20  | E8    | 197 | LEU  |
| 20  | E8    | 201 | LEU  |
| 20  | E8    | 202 | ASP  |
| 20  | E8    | 203 | TRP  |
| 20  | E8    | 207 | LEU  |
| 20  | E8    | 209 | SER  |
| 20  | E8    | 214 | LEU  |
| 20  | E8    | 219 | LEU  |
| 20  | E8    | 308 | GLU  |
| 20  | E8    | 337 | THR  |
| 20  | E8    | 343 | THR  |
| 20  | E8    | 345 | LEU  |
| 20  | E8    | 349 | THR  |
| 20  | E8    | 426 | LEU  |
| 20  | E8    | 436 | THR  |
| 20  | E8    | 437 | SER  |
| 20  | E8    | 454 | MET  |
| 20  | E8    | 494 | ILE  |
| 21  | H     | 124 | LEU  |
| 21  | H     | 138 | GLU  |
| 21  | H     | 228 | LEU  |
| 21  | H     | 320 | SER  |
| 21  | H     | 324 | LEU  |
| 21  | H     | 371 | THR  |
| 22  | I     | 112 | LEU  |
| 22  | I     | 149 | SER  |
| 22  | I     | 189 | LEU  |
| 22  | I     | 286 | LEU  |
| 22  | I     | 300 | LEU  |
| 22  | I     | 340 | GLN  |
| 22  | I     | 371 | THR  |
| 22  | I     | 372 | LEU  |
| 23  | J32   | 579 | ARG  |
| 23  | J32   | 603 | LEU  |
| 23  | J32   | 681 | GLU  |
| 23  | J32   | 686 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | J32   | 722 | LEU  |
| 23  | J32   | 731 | LEU  |
| 23  | J32   | 737 | TRP  |
| 23  | J32   | 739 | SER  |
| 21  | H8    | 124 | LEU  |
| 21  | H8    | 138 | GLU  |
| 21  | H8    | 228 | LEU  |
| 21  | H8    | 320 | SER  |
| 21  | H8    | 324 | LEU  |
| 21  | H8    | 371 | THR  |
| 22  | I8    | 112 | LEU  |
| 22  | I8    | 149 | SER  |
| 22  | I8    | 189 | LEU  |
| 22  | I8    | 272 | TYR  |
| 22  | I8    | 286 | LEU  |
| 22  | I8    | 300 | LEU  |
| 22  | I8    | 340 | GLN  |
| 22  | I8    | 371 | THR  |
| 22  | I8    | 372 | LEU  |
| 23  | J8    | 579 | ARG  |
| 23  | J8    | 603 | LEU  |
| 23  | J8    | 681 | GLU  |
| 23  | J8    | 686 | MET  |
| 23  | J8    | 722 | LEU  |
| 23  | J8    | 731 | LEU  |
| 23  | J8    | 737 | TRP  |
| 23  | J8    | 739 | SER  |
| 21  | H24   | 228 | LEU  |
| 21  | H24   | 320 | SER  |
| 21  | H24   | 324 | LEU  |
| 22  | I24   | 112 | LEU  |
| 22  | I24   | 149 | SER  |
| 22  | I24   | 189 | LEU  |
| 22  | I24   | 272 | TYR  |
| 22  | I24   | 286 | LEU  |
| 22  | I24   | 292 | ASP  |
| 22  | I24   | 300 | LEU  |
| 22  | I24   | 340 | GLN  |
| 22  | I24   | 371 | THR  |
| 22  | I24   | 372 | LEU  |
| 23  | J24   | 579 | ARG  |
| 23  | J24   | 603 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | J24   | 681  | GLU  |
| 23  | J24   | 686  | MET  |
| 23  | J24   | 722  | LEU  |
| 23  | J24   | 731  | LEU  |
| 23  | J24   | 737  | TRP  |
| 23  | J24   | 739  | SER  |
| 21  | H16   | 228  | LEU  |
| 21  | H16   | 320  | SER  |
| 21  | H16   | 324  | LEU  |
| 22  | I16   | 112  | LEU  |
| 22  | I16   | 149  | SER  |
| 22  | I16   | 189  | LEU  |
| 22  | I16   | 272  | TYR  |
| 22  | I16   | 286  | LEU  |
| 22  | I16   | 292  | ASP  |
| 22  | I16   | 300  | LEU  |
| 22  | I16   | 340  | GLN  |
| 22  | I16   | 371  | THR  |
| 22  | I16   | 372  | LEU  |
| 23  | J16   | 579  | ARG  |
| 23  | J16   | 603  | LEU  |
| 23  | J16   | 681  | GLU  |
| 23  | J16   | 686  | MET  |
| 23  | J16   | 722  | LEU  |
| 23  | J16   | 731  | LEU  |
| 23  | J16   | 737  | TRP  |
| 23  | J16   | 739  | SER  |
| 24  | D     | 246  | VAL  |
| 24  | D     | 360  | THR  |
| 24  | D     | 369  | HIS  |
| 24  | D     | 399  | SER  |
| 24  | D     | 624  | SER  |
| 24  | D     | 735  | SER  |
| 24  | D     | 744  | LEU  |
| 24  | D     | 1071 | SER  |
| 24  | D     | 1207 | ASP  |
| 24  | D     | 1258 | TYR  |
| 24  | D     | 1390 | ASP  |
| 24  | D     | 1397 | THR  |
| 24  | D     | 1409 | LEU  |
| 24  | D8    | 246  | VAL  |
| 24  | D8    | 360  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D8    | 369  | HIS  |
| 24  | D8    | 399  | SER  |
| 24  | D8    | 624  | SER  |
| 24  | D8    | 735  | SER  |
| 24  | D8    | 744  | LEU  |
| 24  | D8    | 1071 | SER  |
| 24  | D8    | 1207 | ASP  |
| 24  | D8    | 1258 | TYR  |
| 24  | D8    | 1390 | ASP  |
| 24  | D8    | 1397 | THR  |
| 24  | D8    | 1409 | LEU  |
| 24  | D16   | 139  | GLU  |
| 24  | D16   | 246  | VAL  |
| 24  | D16   | 360  | THR  |
| 24  | D16   | 369  | HIS  |
| 24  | D16   | 399  | SER  |
| 24  | D16   | 538  | PHE  |
| 24  | D16   | 624  | SER  |
| 24  | D16   | 735  | SER  |
| 24  | D16   | 744  | LEU  |
| 24  | D16   | 1071 | SER  |
| 24  | D16   | 1207 | ASP  |
| 24  | D16   | 1258 | TYR  |
| 24  | D16   | 1302 | ASP  |
| 24  | D16   | 1354 | ASP  |
| 24  | D16   | 1390 | ASP  |
| 24  | D16   | 1397 | THR  |
| 24  | D16   | 1409 | LEU  |
| 24  | D24   | 6    | GLU  |
| 24  | D24   | 139  | GLU  |
| 24  | D24   | 246  | VAL  |
| 24  | D24   | 360  | THR  |
| 24  | D24   | 369  | HIS  |
| 24  | D24   | 399  | SER  |
| 24  | D24   | 538  | PHE  |
| 24  | D24   | 624  | SER  |
| 24  | D24   | 735  | SER  |
| 24  | D24   | 744  | LEU  |
| 24  | D24   | 1071 | SER  |
| 24  | D24   | 1207 | ASP  |
| 24  | D24   | 1258 | TYR  |
| 24  | D24   | 1302 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D24   | 1354 | ASP  |
| 24  | D24   | 1390 | ASP  |
| 24  | D24   | 1397 | THR  |
| 24  | D24   | 1409 | LEU  |
| 24  | D32   | 139  | GLU  |
| 24  | D32   | 246  | VAL  |
| 24  | D32   | 360  | THR  |
| 24  | D32   | 369  | HIS  |
| 24  | D32   | 399  | SER  |
| 24  | D32   | 538  | PHE  |
| 24  | D32   | 624  | SER  |
| 24  | D32   | 735  | SER  |
| 24  | D32   | 744  | LEU  |
| 24  | D32   | 1071 | SER  |
| 24  | D32   | 1207 | ASP  |
| 24  | D32   | 1258 | TYR  |
| 24  | D32   | 1302 | ASP  |
| 24  | D32   | 1354 | ASP  |
| 24  | D32   | 1390 | ASP  |
| 24  | D32   | 1397 | THR  |
| 24  | D32   | 1409 | LEU  |
| 24  | D40   | 139  | GLU  |
| 24  | D40   | 246  | VAL  |
| 24  | D40   | 360  | THR  |
| 24  | D40   | 369  | HIS  |
| 24  | D40   | 399  | SER  |
| 24  | D40   | 538  | PHE  |
| 24  | D40   | 624  | SER  |
| 24  | D40   | 735  | SER  |
| 24  | D40   | 744  | LEU  |
| 24  | D40   | 1071 | SER  |
| 24  | D40   | 1207 | ASP  |
| 24  | D40   | 1258 | TYR  |
| 24  | D40   | 1302 | ASP  |
| 24  | D40   | 1354 | ASP  |
| 24  | D40   | 1390 | ASP  |
| 24  | D40   | 1397 | THR  |
| 24  | D40   | 1409 | LEU  |
| 10  | C32   | 71   | SER  |
| 10  | C32   | 89   | LEU  |
| 10  | C32   | 98   | LEU  |
| 10  | C32   | 105  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C32   | 124 | TYR  |
| 10  | C32   | 156 | GLN  |
| 10  | C32   | 179 | ASN  |
| 10  | C32   | 180 | ARG  |
| 10  | C32   | 184 | THR  |
| 10  | C32   | 202 | LEU  |
| 10  | C32   | 248 | LEU  |
| 10  | C32   | 249 | THR  |
| 10  | C32   | 279 | LEU  |
| 10  | C32   | 280 | SER  |
| 10  | C32   | 284 | SER  |
| 10  | C32   | 294 | THR  |
| 10  | C32   | 303 | SER  |
| 10  | C32   | 308 | THR  |
| 10  | C32   | 313 | ILE  |
| 10  | C32   | 334 | MET  |
| 10  | C32   | 339 | THR  |
| 10  | C32   | 342 | THR  |
| 10  | C32   | 343 | THR  |
| 10  | C32   | 345 | MET  |
| 10  | C32   | 365 | LEU  |
| 10  | C32   | 379 | GLU  |
| 10  | C32   | 389 | LEU  |
| 10  | C32   | 415 | SER  |
| 10  | C32   | 422 | THR  |
| 10  | C32   | 423 | SER  |
| 10  | C32   | 424 | ASP  |
| 10  | C32   | 426 | LEU  |
| 10  | C32   | 427 | ASP  |
| 10  | C32   | 432 | THR  |
| 10  | C32   | 447 | PHE  |
| 10  | C32   | 450 | PRO  |
| 10  | C32   | 454 | SER  |
| 10  | C32   | 459 | LEU  |
| 10  | C32   | 461 | THR  |
| 10  | C32   | 485 | THR  |
| 10  | C32   | 499 | LEU  |
| 10  | C32   | 516 | CYS  |
| 10  | C32   | 528 | LEU  |
| 10  | C32   | 530 | THR  |
| 10  | C32   | 555 | LYS  |
| 10  | C32   | 563 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C32   | 572  | ILE  |
| 10  | C32   | 605  | GLU  |
| 10  | C32   | 619  | LEU  |
| 10  | C32   | 625  | SER  |
| 10  | C32   | 634  | SER  |
| 10  | C32   | 639  | MET  |
| 10  | C32   | 670  | GLU  |
| 10  | C32   | 672  | ASP  |
| 10  | C32   | 685  | CYS  |
| 10  | C32   | 703  | SER  |
| 10  | C32   | 716  | THR  |
| 10  | C32   | 721  | PHE  |
| 10  | C32   | 724  | SER  |
| 10  | C32   | 725  | LEU  |
| 10  | C32   | 727  | THR  |
| 10  | C32   | 728  | SER  |
| 10  | C32   | 730  | LEU  |
| 10  | C32   | 732  | THR  |
| 10  | C32   | 734  | LEU  |
| 10  | C32   | 749  | LEU  |
| 10  | C32   | 753  | LEU  |
| 10  | C32   | 764  | ILE  |
| 10  | C32   | 798  | VAL  |
| 10  | C32   | 805  | LEU  |
| 10  | C32   | 814  | SER  |
| 10  | C32   | 827  | VAL  |
| 10  | C32   | 849  | SER  |
| 10  | C32   | 851  | LEU  |
| 10  | C32   | 866  | SER  |
| 10  | C32   | 879  | LEU  |
| 10  | C32   | 911  | ILE  |
| 10  | C32   | 984  | SER  |
| 10  | C32   | 994  | LEU  |
| 10  | C32   | 996  | THR  |
| 10  | C32   | 1006 | SER  |
| 10  | C32   | 1036 | SER  |
| 10  | C32   | 1041 | LEU  |
| 10  | C32   | 1049 | SER  |
| 10  | C32   | 1050 | HIS  |
| 10  | C32   | 1057 | THR  |
| 10  | C32   | 1068 | THR  |
| 10  | C32   | 1079 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C32   | 1081 | SER  |
| 10  | C32   | 1083 | SER  |
| 10  | C32   | 1085 | SER  |
| 10  | C32   | 1105 | LEU  |
| 10  | C32   | 1112 | LEU  |
| 10  | C32   | 1117 | LEU  |
| 10  | C32   | 1127 | THR  |
| 10  | C32   | 1132 | SER  |
| 10  | C32   | 1157 | LEU  |
| 10  | C32   | 1158 | HIS  |
| 10  | C32   | 1163 | LEU  |
| 10  | C32   | 1166 | SER  |
| 10  | C32   | 1173 | LEU  |
| 10  | C32   | 1208 | SER  |
| 10  | C32   | 1219 | ILE  |
| 10  | C32   | 1240 | SER  |
| 10  | C32   | 1275 | LEU  |
| 10  | C32   | 1277 | SER  |
| 10  | C32   | 1283 | LEU  |
| 10  | C32   | 1293 | THR  |
| 10  | C32   | 1309 | ARG  |
| 10  | C32   | 1341 | THR  |
| 10  | C32   | 1358 | ASP  |
| 10  | C32   | 1363 | ASP  |
| 10  | C32   | 1385 | LEU  |
| 10  | C32   | 1393 | SER  |
| 10  | C32   | 1445 | THR  |
| 10  | C32   | 1447 | LEU  |
| 10  | C32   | 1448 | LEU  |
| 10  | C32   | 1504 | ASP  |
| 10  | C32   | 1505 | MET  |
| 10  | C32   | 1507 | LEU  |
| 10  | C32   | 1538 | THR  |
| 10  | C32   | 1560 | GLN  |
| 10  | C32   | 1614 | LEU  |
| 10  | C32   | 1622 | SER  |
| 10  | C32   | 1624 | LEU  |
| 10  | C32   | 1628 | SER  |
| 10  | C32   | 1657 | SER  |
| 10  | C32   | 1658 | ASP  |
| 10  | C32   | 1661 | LEU  |
| 10  | C32   | 1665 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C32   | 1667 | LEU  |
| 10  | C32   | 1673 | LEU  |
| 10  | C32   | 1674 | LEU  |
| 10  | C32   | 1695 | LEU  |
| 10  | C32   | 1703 | ILE  |
| 10  | C32   | 1754 | LEU  |
| 10  | C32   | 1772 | ASP  |
| 10  | C32   | 1791 | GLN  |
| 10  | C32   | 1794 | THR  |
| 10  | C32   | 1827 | THR  |
| 10  | C32   | 1828 | THR  |
| 10  | C32   | 1832 | MET  |
| 12  | A48   | 106  | GLN  |
| 12  | A48   | 156  | MET  |
| 12  | A48   | 160  | THR  |
| 12  | A48   | 242  | THR  |
| 12  | A48   | 309  | VAL  |
| 12  | A48   | 333  | SER  |
| 12  | A48   | 334  | THR  |
| 12  | A48   | 438  | ARG  |
| 12  | A48   | 443  | LEU  |
| 12  | A48   | 466  | SER  |
| 12  | A48   | 467  | SER  |
| 12  | A48   | 524  | GLU  |
| 12  | A48   | 585  | MET  |
| 12  | A48   | 760  | LEU  |
| 12  | A48   | 835  | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (312) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R     | 82   | ASN  |
| 1   | R     | 265  | GLN  |
| 1   | R     | 498  | ASN  |
| 1   | R     | 516  | ASN  |
| 1   | R     | 529  | HIS  |
| 1   | R     | 785  | ASN  |
| 1   | R     | 909  | GLN  |
| 1   | R     | 1042 | ASN  |
| 1   | R     | 1122 | HIS  |
| 1   | R     | 1149 | HIS  |
| 1   | R     | 1166 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | R     | 1360 | GLN  |
| 1   | R     | 1398 | GLN  |
| 1   | R     | 1472 | HIS  |
| 1   | R     | 1473 | HIS  |
| 2   | M     | 218  | ASN  |
| 2   | M     | 271  | GLN  |
| 2   | M     | 310  | HIS  |
| 2   | M     | 311  | GLN  |
| 2   | M     | 438  | GLN  |
| 2   | M     | 468  | HIS  |
| 2   | M     | 534  | HIS  |
| 2   | M     | 593  | HIS  |
| 2   | M     | 602  | GLN  |
| 2   | M     | 606  | GLN  |
| 2   | M     | 618  | HIS  |
| 2   | M     | 639  | GLN  |
| 2   | M     | 813  | ASN  |
| 3   | N     | 4    | GLN  |
| 3   | N     | 43   | ASN  |
| 3   | N     | 97   | HIS  |
| 3   | N     | 107  | ASN  |
| 3   | N     | 114  | HIS  |
| 1   | R8    | 265  | GLN  |
| 1   | R8    | 303  | ASN  |
| 1   | R8    | 516  | ASN  |
| 1   | R8    | 529  | HIS  |
| 1   | R8    | 785  | ASN  |
| 1   | R8    | 909  | GLN  |
| 1   | R8    | 1042 | ASN  |
| 1   | R8    | 1122 | HIS  |
| 1   | R8    | 1149 | HIS  |
| 1   | R8    | 1166 | ASN  |
| 1   | R8    | 1379 | GLN  |
| 1   | R8    | 1398 | GLN  |
| 1   | R8    | 1472 | HIS  |
| 1   | R8    | 1473 | HIS  |
| 2   | M8    | 218  | ASN  |
| 2   | M8    | 236  | GLN  |
| 2   | M8    | 271  | GLN  |
| 2   | M8    | 310  | HIS  |
| 2   | M8    | 438  | GLN  |
| 2   | M8    | 468  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M8    | 534 | HIS  |
| 2   | M8    | 576 | HIS  |
| 2   | M8    | 593 | HIS  |
| 2   | M8    | 602 | GLN  |
| 2   | M8    | 606 | GLN  |
| 2   | M8    | 618 | HIS  |
| 2   | M8    | 639 | GLN  |
| 2   | M8    | 766 | ASN  |
| 2   | M8    | 813 | ASN  |
| 3   | N8    | 4   | GLN  |
| 3   | N8    | 89  | ASN  |
| 3   | N8    | 97  | HIS  |
| 3   | N8    | 107 | ASN  |
| 3   | N8    | 114 | HIS  |
| 4   | T     | 160 | HIS  |
| 4   | T     | 248 | GLN  |
| 4   | T     | 258 | ASN  |
| 4   | T     | 353 | GLN  |
| 4   | T     | 653 | GLN  |
| 4   | T8    | 160 | HIS  |
| 4   | T8    | 248 | GLN  |
| 4   | T8    | 258 | ASN  |
| 4   | T8    | 264 | GLN  |
| 4   | T8    | 353 | GLN  |
| 4   | T8    | 653 | GLN  |
| 5   | P     | 254 | HIS  |
| 5   | P     | 366 | HIS  |
| 5   | P     | 385 | GLN  |
| 5   | P     | 467 | GLN  |
| 5   | P     | 506 | ASN  |
| 5   | P     | 507 | GLN  |
| 5   | P     | 593 | GLN  |
| 5   | P     | 615 | HIS  |
| 5   | P     | 624 | HIS  |
| 5   | P     | 641 | GLN  |
| 5   | P     | 649 | HIS  |
| 5   | P     | 676 | GLN  |
| 6   | O     | 105 | ASN  |
| 6   | O     | 154 | GLN  |
| 7   | Q     | 27  | GLN  |
| 7   | Q     | 57  | ASN  |
| 7   | Q     | 62  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | Q     | 216  | GLN  |
| 7   | Q     | 334  | ASN  |
| 5   | P8    | 123  | GLN  |
| 5   | P8    | 254  | HIS  |
| 5   | P8    | 366  | HIS  |
| 5   | P8    | 385  | GLN  |
| 5   | P8    | 467  | GLN  |
| 5   | P8    | 506  | ASN  |
| 5   | P8    | 507  | GLN  |
| 5   | P8    | 641  | GLN  |
| 5   | P8    | 649  | HIS  |
| 5   | P8    | 676  | GLN  |
| 7   | Q8    | 27   | GLN  |
| 7   | Q8    | 57   | ASN  |
| 7   | Q8    | 62   | HIS  |
| 7   | Q8    | 216  | GLN  |
| 7   | Q8    | 334  | ASN  |
| 8   | L     | 186  | GLN  |
| 8   | L     | 294  | HIS  |
| 8   | L     | 495  | GLN  |
| 8   | L     | 507  | HIS  |
| 8   | L     | 564  | HIS  |
| 8   | L     | 601  | HIS  |
| 8   | L     | 645  | HIS  |
| 8   | L     | 705  | GLN  |
| 8   | L     | 738  | HIS  |
| 8   | L     | 740  | ASN  |
| 8   | L     | 762  | HIS  |
| 8   | L     | 789  | ASN  |
| 8   | L     | 850  | ASN  |
| 8   | L     | 1054 | HIS  |
| 8   | L8    | 289  | ASN  |
| 8   | L8    | 294  | HIS  |
| 8   | L8    | 295  | HIS  |
| 8   | L8    | 507  | HIS  |
| 8   | L8    | 564  | HIS  |
| 8   | L8    | 634  | HIS  |
| 8   | L8    | 645  | HIS  |
| 8   | L8    | 738  | HIS  |
| 8   | L8    | 740  | ASN  |
| 8   | L8    | 762  | HIS  |
| 8   | L8    | 789  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L8    | 850  | ASN  |
| 8   | L8    | 1054 | HIS  |
| 9   | K     | 577  | GLN  |
| 9   | K     | 655  | GLN  |
| 9   | K     | 786  | GLN  |
| 9   | K     | 867  | HIS  |
| 9   | K     | 998  | GLN  |
| 9   | K     | 1020 | HIS  |
| 9   | K     | 1027 | HIS  |
| 9   | K     | 1032 | HIS  |
| 9   | K     | 1110 | GLN  |
| 9   | K     | 1173 | ASN  |
| 9   | K     | 1220 | ASN  |
| 9   | K8    | 577  | GLN  |
| 9   | K8    | 655  | GLN  |
| 9   | K8    | 786  | GLN  |
| 9   | K8    | 1027 | HIS  |
| 9   | K8    | 1032 | HIS  |
| 9   | K8    | 1110 | GLN  |
| 9   | K8    | 1173 | ASN  |
| 9   | K8    | 1220 | ASN  |
| 12  | A     | 302  | GLN  |
| 12  | A     | 348  | GLN  |
| 12  | A     | 432  | GLN  |
| 12  | A     | 520  | HIS  |
| 12  | A     | 615  | GLN  |
| 12  | A     | 668  | HIS  |
| 13  | V     | 790  | GLN  |
| 13  | V     | 899  | HIS  |
| 13  | V     | 919  | GLN  |
| 14  | W     | 49   | GLN  |
| 14  | W     | 230  | HIS  |
| 14  | W     | 310  | ASN  |
| 14  | W     | 388  | GLN  |
| 14  | W     | 645  | HIS  |
| 14  | W     | 688  | HIS  |
| 14  | W     | 705  | HIS  |
| 14  | W     | 762  | GLN  |
| 15  | J     | 564  | GLN  |
| 15  | J     | 664  | GLN  |
| 15  | J     | 675  | ASN  |
| 10  | C     | 31   | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C     | 41   | GLN  |
| 10  | C     | 75   | GLN  |
| 10  | C     | 328  | HIS  |
| 10  | C     | 456  | ASN  |
| 10  | C     | 470  | HIS  |
| 10  | C     | 490  | GLN  |
| 10  | C     | 529  | GLN  |
| 10  | C     | 559  | ASN  |
| 10  | C     | 731  | GLN  |
| 10  | C     | 758  | GLN  |
| 10  | C     | 836  | GLN  |
| 10  | C     | 934  | HIS  |
| 10  | C     | 969  | ASN  |
| 10  | C     | 993  | HIS  |
| 10  | C     | 1158 | HIS  |
| 10  | C     | 1332 | GLN  |
| 10  | C     | 1366 | GLN  |
| 10  | C     | 1424 | GLN  |
| 10  | C     | 1626 | GLN  |
| 10  | C     | 1650 | ASN  |
| 10  | C     | 1721 | GLN  |
| 10  | C     | 1788 | HIS  |
| 10  | C8    | 31   | HIS  |
| 10  | C8    | 35   | ASN  |
| 10  | C8    | 41   | GLN  |
| 10  | C8    | 75   | GLN  |
| 10  | C8    | 328  | HIS  |
| 10  | C8    | 470  | HIS  |
| 10  | C8    | 490  | GLN  |
| 10  | C8    | 758  | GLN  |
| 10  | C8    | 815  | GLN  |
| 10  | C8    | 817  | HIS  |
| 10  | C8    | 836  | GLN  |
| 10  | C8    | 934  | HIS  |
| 10  | C8    | 963  | GLN  |
| 10  | C8    | 1158 | HIS  |
| 10  | C8    | 1197 | GLN  |
| 10  | C8    | 1332 | GLN  |
| 10  | C8    | 1366 | GLN  |
| 10  | C8    | 1424 | GLN  |
| 10  | C8    | 1626 | GLN  |
| 10  | C8    | 1650 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | C8    | 1721 | GLN  |
| 18  | B     | 75   | HIS  |
| 18  | B     | 268  | GLN  |
| 18  | B     | 390  | HIS  |
| 18  | B     | 410  | GLN  |
| 18  | B     | 847  | GLN  |
| 18  | B     | 923  | GLN  |
| 18  | B     | 960  | GLN  |
| 18  | B     | 1004 | GLN  |
| 18  | B     | 1016 | HIS  |
| 18  | B     | 1032 | GLN  |
| 18  | B     | 1212 | GLN  |
| 18  | B     | 1264 | GLN  |
| 18  | B     | 1343 | HIS  |
| 18  | B     | 1543 | HIS  |
| 18  | B     | 1575 | GLN  |
| 18  | B     | 1727 | HIS  |
| 18  | B     | 1745 | HIS  |
| 18  | B     | 1748 | HIS  |
| 18  | B     | 1772 | HIS  |
| 18  | B     | 1871 | GLN  |
| 18  | B     | 1901 | GLN  |
| 18  | B8    | 75   | HIS  |
| 18  | B8    | 268  | GLN  |
| 18  | B8    | 390  | HIS  |
| 18  | B8    | 410  | GLN  |
| 18  | B8    | 847  | GLN  |
| 18  | B8    | 923  | GLN  |
| 18  | B8    | 960  | GLN  |
| 18  | B8    | 1004 | GLN  |
| 18  | B8    | 1016 | HIS  |
| 18  | B8    | 1032 | GLN  |
| 18  | B8    | 1212 | GLN  |
| 18  | B8    | 1264 | GLN  |
| 18  | B8    | 1343 | HIS  |
| 18  | B8    | 1543 | HIS  |
| 18  | B8    | 1575 | GLN  |
| 18  | B8    | 1727 | HIS  |
| 18  | B8    | 1745 | HIS  |
| 18  | B8    | 1748 | HIS  |
| 18  | B8    | 1772 | HIS  |
| 18  | B8    | 1871 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | B8    | 1901 | GLN  |
| 19  | 4     | 244  | GLN  |
| 20  | E     | 236  | HIS  |
| 20  | E     | 238  | HIS  |
| 20  | E     | 382  | HIS  |
| 20  | E     | 509  | GLN  |
| 19  | 48    | 244  | GLN  |
| 19  | 48    | 337  | HIS  |
| 20  | E8    | 236  | HIS  |
| 20  | E8    | 238  | HIS  |
| 20  | E8    | 382  | HIS  |
| 20  | E8    | 509  | GLN  |
| 21  | H     | 148  | GLN  |
| 21  | H     | 195  | GLN  |
| 21  | H     | 231  | HIS  |
| 21  | H     | 312  | GLN  |
| 21  | H     | 339  | GLN  |
| 22  | I     | 162  | GLN  |
| 22  | I     | 179  | HIS  |
| 22  | I     | 203  | GLN  |
| 21  | H8    | 148  | GLN  |
| 21  | H8    | 195  | GLN  |
| 21  | H8    | 231  | HIS  |
| 21  | H8    | 312  | GLN  |
| 21  | H8    | 339  | GLN  |
| 22  | I8    | 139  | GLN  |
| 22  | I8    | 162  | GLN  |
| 22  | I8    | 179  | HIS  |
| 22  | I8    | 203  | GLN  |
| 23  | J8    | 596  | GLN  |
| 23  | J8    | 650  | GLN  |
| 24  | D     | 45   | HIS  |
| 24  | D     | 176  | GLN  |
| 24  | D     | 308  | ASN  |
| 24  | D     | 374  | ASN  |
| 24  | D     | 406  | ASN  |
| 24  | D     | 528  | HIS  |
| 24  | D     | 654  | HIS  |
| 24  | D     | 810  | HIS  |
| 24  | D     | 833  | HIS  |
| 24  | D8    | 45   | HIS  |
| 24  | D8    | 176  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | D8    | 528  | HIS  |
| 24  | D8    | 654  | HIS  |
| 24  | D8    | 833  | HIS  |
| 24  | D8    | 1017 | GLN  |
| 24  | D8    | 1100 | GLN  |
| 24  | D8    | 1138 | GLN  |
| 24  | D8    | 1328 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 10  | C16   | 17               |
| 10  | C24   | 17               |
| 10  | C     | 17               |
| 10  | C32   | 17               |
| 10  | C8    | 15               |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9   | K     | 9                |
| 9   | K8    | 9                |
| 18  | B8    | 7                |
| 18  | B     | 6                |
| 11  | A24   | 5                |
| 11  | A40   | 5                |
| 11  | A16   | 5                |
| 11  | A32   | 5                |
| 19  | 4     | 5                |
| 19  | 48    | 5                |
| 1   | R     | 4                |
| 1   | R8    | 4                |
| 1   | R16   | 4                |
| 14  | W     | 4                |
| 12  | A     | 4                |
| 12  | A48   | 4                |
| 20  | E     | 3                |
| 20  | E8    | 3                |
| 5   | P     | 3                |
| 5   | P8    | 3                |
| 5   | P16   | 3                |
| 13  | V     | 3                |
| 22  | I     | 2                |
| 22  | I8    | 2                |
| 22  | I24   | 2                |
| 22  | I16   | 2                |
| 7   | Q     | 2                |
| 7   | Q8    | 2                |
| 7   | Q16   | 2                |
| 3   | N     | 2                |
| 3   | N8    | 2                |
| 3   | N16   | 2                |
| 15  | J     | 1                |
| 23  | J32   | 1                |
| 23  | J8    | 1                |
| 23  | J24   | 1                |
| 23  | J16   | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I     | 210:LYS   | C      | 252:ARG   | N      | 22.49        |
| 1     | I8    | 210:LYS   | C      | 252:ARG   | N      | 22.49        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I24   | 210:LYS   | C      | 252:ARG   | N      | 22.49        |
| 1     | I16   | 210:LYS   | C      | 252:ARG   | N      | 22.49        |
| 1     | R     | 1121:ARG  | C      | 1122:HIS  | N      | 1.87         |
| 1     | R8    | 1121:ARG  | C      | 1122:HIS  | N      | 1.87         |
| 1     | R16   | 1121:ARG  | C      | 1122:HIS  | N      | 1.87         |
| 1     | C16   | 668:ALA   | C      | 669:GLY   | N      | 1.83         |
| 1     | C24   | 668:ALA   | C      | 669:GLY   | N      | 1.83         |
| 1     | C     | 668:ALA   | C      | 669:GLY   | N      | 1.83         |
| 1     | C8    | 668:ALA   | C      | 669:GLY   | N      | 1.83         |
| 1     | C32   | 668:ALA   | C      | 669:GLY   | N      | 1.83         |
| 1     | K     | 719:GLY   | C      | 720:SER   | N      | 1.74         |
| 1     | K8    | 719:GLY   | C      | 720:SER   | N      | 1.74         |
| 1     | C16   | 670:GLU   | C      | 671:LYS   | N      | 1.67         |
| 1     | C24   | 670:GLU   | C      | 671:LYS   | N      | 1.67         |
| 1     | C     | 670:GLU   | C      | 671:LYS   | N      | 1.67         |
| 1     | C8    | 670:GLU   | C      | 671:LYS   | N      | 1.67         |
| 1     | E     | 340:GLY   | C      | 341:TYR   | N      | 1.67         |
| 1     | E8    | 340:GLY   | C      | 341:TYR   | N      | 1.67         |
| 1     | C32   | 670:GLU   | C      | 671:LYS   | N      | 1.67         |
| 1     | W     | 584:CYS   | C      | 585:ILE   | N      | 1.66         |
| 1     | E     | 429:PRO   | C      | 430:ALA   | N      | 1.63         |
| 1     | E8    | 429:PRO   | C      | 430:ALA   | N      | 1.63         |
| 1     | K     | 1273:GLU  | C      | 1274:GLY  | N      | 1.61         |
| 1     | K8    | 1273:GLU  | C      | 1274:GLY  | N      | 1.61         |
| 1     | R     | 1185:THR  | C      | 1186:THR  | N      | 1.20         |
| 1     | R     | 1224:VAL  | C      | 1225:PHE  | N      | 1.20         |
| 1     | R8    | 1185:THR  | C      | 1186:THR  | N      | 1.20         |
| 1     | R8    | 1224:VAL  | C      | 1225:PHE  | N      | 1.20         |
| 1     | R16   | 1185:THR  | C      | 1186:THR  | N      | 1.20         |
| 1     | R16   | 1224:VAL  | C      | 1225:PHE  | N      | 1.20         |
| 1     | P     | 14:VAL    | C      | 15:LEU    | N      | 1.20         |
| 1     | P     | 392:PRO   | C      | 393:VAL   | N      | 1.20         |
| 1     | P8    | 14:VAL    | C      | 15:LEU    | N      | 1.20         |
| 1     | P8    | 392:PRO   | C      | 393:VAL   | N      | 1.20         |
| 1     | P16   | 14:VAL    | C      | 15:LEU    | N      | 1.20         |
| 1     | P16   | 392:PRO   | C      | 393:VAL   | N      | 1.20         |
| 1     | K     | 650:THR   | C      | 651:VAL   | N      | 1.20         |
| 1     | C16   | 105:TRP   | C      | 106:GLY   | N      | 1.20         |
| 1     | C16   | 1659:ASP  | C      | 1660:SER  | N      | 1.20         |
| 1     | C16   | 1732:LYS  | C      | 1733:ARG  | N      | 1.20         |
| 1     | C24   | 105:TRP   | C      | 106:GLY   | N      | 1.20         |
| 1     | C24   | 1659:ASP  | C      | 1660:SER  | N      | 1.20         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C24   | 1732:LYS  | C      | 1733:ARG  | N      | 1.20         |
| 1     | V     | 830:GLN   | C      | 831:LYS   | N      | 1.20         |
| 1     | J     | 595:THR   | C      | 596:GLN   | N      | 1.20         |
| 1     | C     | 105:TRP   | C      | 106:GLY   | N      | 1.20         |
| 1     | C     | 1659:ASP  | C      | 1660:SER  | N      | 1.20         |
| 1     | C     | 1732:LYS  | C      | 1733:ARG  | N      | 1.20         |
| 1     | C8    | 105:TRP   | C      | 106:GLY   | N      | 1.20         |
| 1     | C8    | 1732:LYS  | C      | 1733:ARG  | N      | 1.20         |
| 1     | B     | 1685:THR  | C      | 1686:SER  | N      | 1.20         |
| 1     | B     | 1838:ALA  | C      | 1839:GLU  | N      | 1.20         |
| 1     | B8    | 442:SER   | C      | 443:PHE   | N      | 1.20         |
| 1     | B8    | 1685:THR  | C      | 1686:SER  | N      | 1.20         |
| 1     | B8    | 1745:HIS  | C      | 1746:ILE  | N      | 1.20         |
| 1     | I8    | 147:SER   | C      | 148:VAL   | N      | 1.20         |
| 1     | I24   | 147:SER   | C      | 148:VAL   | N      | 1.20         |
| 1     | I16   | 147:SER   | C      | 148:VAL   | N      | 1.20         |
| 1     | C32   | 105:TRP   | C      | 106:GLY   | N      | 1.20         |
| 1     | C32   | 1659:ASP  | C      | 1660:SER  | N      | 1.20         |
| 1     | C32   | 1732:LYS  | C      | 1733:ARG  | N      | 1.20         |
| 1     | Q     | 164:ASN   | C      | 165:GLY   | N      | 1.19         |
| 1     | Q     | 222:PHE   | C      | 223:GLN   | N      | 1.19         |
| 1     | Q8    | 164:ASN   | C      | 165:GLY   | N      | 1.19         |
| 1     | Q8    | 222:PHE   | C      | 223:GLN   | N      | 1.19         |
| 1     | Q16   | 164:ASN   | C      | 165:GLY   | N      | 1.19         |
| 1     | Q16   | 222:PHE   | C      | 223:GLN   | N      | 1.19         |
| 1     | K     | 677:GLU   | C      | 678:GLU   | N      | 1.19         |
| 1     | K8    | 650:THR   | C      | 651:VAL   | N      | 1.19         |
| 1     | K8    | 677:GLU   | C      | 678:GLU   | N      | 1.19         |
| 1     | C16   | 2:VAL     | C      | 3:SER     | N      | 1.19         |
| 1     | C16   | 561:ASN   | C      | 562:PRO   | N      | 1.19         |
| 1     | C16   | 1777:SER  | C      | 1778:ASN  | N      | 1.19         |
| 1     | A24   | 57:PRO    | C      | 58:SER    | N      | 1.19         |
| 1     | A24   | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | C24   | 2:VAL     | C      | 3:SER     | N      | 1.19         |
| 1     | C24   | 561:ASN   | C      | 562:PRO   | N      | 1.19         |
| 1     | C24   | 1777:SER  | C      | 1778:ASN  | N      | 1.19         |
| 1     | A40   | 57:PRO    | C      | 58:SER    | N      | 1.19         |
| 1     | A40   | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | A     | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | W     | 615:GLU   | C      | 616:GLY   | N      | 1.19         |
| 1     | C     | 2:VAL     | C      | 3:SER     | N      | 1.19         |
| 1     | C     | 561:ASN   | C      | 562:PRO   | N      | 1.19         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 1777:SER  | C      | 1778:ASN  | N      | 1.19         |
| 1     | C8    | 2:VAL     | C      | 3:SER     | N      | 1.19         |
| 1     | C8    | 561:ASN   | C      | 562:PRO   | N      | 1.19         |
| 1     | C8    | 1777:SER  | C      | 1778:ASN  | N      | 1.19         |
| 1     | A16   | 57:PRO    | C      | 58:SER    | N      | 1.19         |
| 1     | A16   | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | A32   | 57:PRO    | C      | 58:SER    | N      | 1.19         |
| 1     | A32   | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | B     | 524:GLU   | C      | 525:GLY   | N      | 1.19         |
| 1     | B     | 1591:MET  | C      | 1592:GLU  | N      | 1.19         |
| 1     | B     | 1903:THR  | C      | 1904:GLU  | N      | 1.19         |
| 1     | B8    | 1591:MET  | C      | 1592:GLU  | N      | 1.19         |
| 1     | B8    | 1903:THR  | C      | 1904:GLU  | N      | 1.19         |
| 1     | 4     | 53:SER    | C      | 54:LEU    | N      | 1.19         |
| 1     | 4     | 207:LEU   | C      | 208:ARG   | N      | 1.19         |
| 1     | E     | 305:GLU   | C      | 306:SER   | N      | 1.19         |
| 1     | 48    | 53:SER    | C      | 54:LEU    | N      | 1.19         |
| 1     | 48    | 207:LEU   | C      | 208:ARG   | N      | 1.19         |
| 1     | E8    | 305:GLU   | C      | 306:SER   | N      | 1.19         |
| 1     | I     | 147:SER   | C      | 148:VAL   | N      | 1.19         |
| 1     | J32   | 716:ARG   | C      | 717:ILE   | N      | 1.19         |
| 1     | J8    | 716:ARG   | C      | 717:ILE   | N      | 1.19         |
| 1     | J24   | 716:ARG   | C      | 717:ILE   | N      | 1.19         |
| 1     | J16   | 716:ARG   | C      | 717:ILE   | N      | 1.19         |
| 1     | C32   | 2:VAL     | C      | 3:SER     | N      | 1.19         |
| 1     | C32   | 561:ASN   | C      | 562:PRO   | N      | 1.19         |
| 1     | C32   | 1777:SER  | C      | 1778:ASN  | N      | 1.19         |
| 1     | A48   | 796:ASP   | C      | 797:VAL   | N      | 1.19         |
| 1     | K     | 713:ASN   | C      | 714:ARG   | N      | 1.18         |
| 1     | K     | 1181:ASP  | C      | 1182:ARG  | N      | 1.18         |
| 1     | K     | 1218:ARG  | C      | 1219:VAL  | N      | 1.18         |
| 1     | K8    | 713:ASN   | C      | 714:ARG   | N      | 1.18         |
| 1     | K8    | 1181:ASP  | C      | 1182:ARG  | N      | 1.18         |
| 1     | K8    | 1218:ARG  | C      | 1219:VAL  | N      | 1.18         |
| 1     | C16   | 438:PRO   | C      | 439:LEU   | N      | 1.18         |
| 1     | C16   | 1287:MET  | C      | 1288:VAL  | N      | 1.18         |
| 1     | C16   | 1332:GLN  | C      | 1333:HIS  | N      | 1.18         |
| 1     | C16   | 1357:LEU  | C      | 1358:ASP  | N      | 1.18         |
| 1     | A24   | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | C24   | 438:PRO   | C      | 439:LEU   | N      | 1.18         |
| 1     | C24   | 1287:MET  | C      | 1288:VAL  | N      | 1.18         |
| 1     | C24   | 1332:GLN  | C      | 1333:HIS  | N      | 1.18         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C24   | 1357:LEU  | C      | 1358:ASP  | N      | 1.18         |
| 1     | A40   | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | A     | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | C     | 438:PRO   | C      | 439:LEU   | N      | 1.18         |
| 1     | C     | 1287:MET  | C      | 1288:VAL  | N      | 1.18         |
| 1     | C     | 1332:GLN  | C      | 1333:HIS  | N      | 1.18         |
| 1     | C     | 1357:LEU  | C      | 1358:ASP  | N      | 1.18         |
| 1     | C8    | 438:PRO   | C      | 439:LEU   | N      | 1.18         |
| 1     | C8    | 1287:MET  | C      | 1288:VAL  | N      | 1.18         |
| 1     | C8    | 1332:GLN  | C      | 1333:HIS  | N      | 1.18         |
| 1     | C8    | 1357:LEU  | C      | 1358:ASP  | N      | 1.18         |
| 1     | A16   | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | A32   | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | B     | 1858:GLU  | C      | 1859:LEU  | N      | 1.18         |
| 1     | B8    | 524:GLU   | C      | 525:GLY   | N      | 1.18         |
| 1     | B8    | 1858:GLU  | C      | 1859:LEU  | N      | 1.18         |
| 1     | 4     | 189:LEU   | C      | 190:ARG   | N      | 1.18         |
| 1     | 48    | 189:LEU   | C      | 190:ARG   | N      | 1.18         |
| 1     | C32   | 438:PRO   | C      | 439:LEU   | N      | 1.18         |
| 1     | C32   | 1287:MET  | C      | 1288:VAL  | N      | 1.18         |
| 1     | C32   | 1332:GLN  | C      | 1333:HIS  | N      | 1.18         |
| 1     | C32   | 1357:LEU  | C      | 1358:ASP  | N      | 1.18         |
| 1     | A48   | 846:HIS   | C      | 847:ARG   | N      | 1.18         |
| 1     | N     | 161:ALA   | C      | 162:THR   | N      | 1.17         |
| 1     | N8    | 161:ALA   | C      | 162:THR   | N      | 1.17         |
| 1     | N16   | 161:ALA   | C      | 162:THR   | N      | 1.17         |
| 1     | P     | 292:GLU   | C      | 293:ASP   | N      | 1.17         |
| 1     | P8    | 292:GLU   | C      | 293:ASP   | N      | 1.17         |
| 1     | P16   | 292:GLU   | C      | 293:ASP   | N      | 1.17         |
| 1     | C16   | 1627:GLY  | C      | 1628:SER  | N      | 1.17         |
| 1     | C16   | 1661:LEU  | C      | 1662:ASP  | N      | 1.17         |
| 1     | A24   | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A24   | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | C24   | 1627:GLY  | C      | 1628:SER  | N      | 1.17         |
| 1     | C24   | 1661:LEU  | C      | 1662:ASP  | N      | 1.17         |
| 1     | A40   | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A40   | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | A     | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A     | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | V     | 807:LYS   | C      | 808:LYS   | N      | 1.17         |
| 1     | C     | 1627:GLY  | C      | 1628:SER  | N      | 1.17         |
| 1     | C     | 1661:LEU  | C      | 1662:ASP  | N      | 1.17         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C8    | 1627:GLY  | C      | 1628:SER  | N      | 1.17         |
| 1     | A16   | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A16   | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | A32   | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A32   | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | 4     | 185:GLY   | C      | 186:GLY   | N      | 1.17         |
| 1     | 48    | 185:GLY   | C      | 186:GLY   | N      | 1.17         |
| 1     | C32   | 1627:GLY  | C      | 1628:SER  | N      | 1.17         |
| 1     | C32   | 1661:LEU  | C      | 1662:ASP  | N      | 1.17         |
| 1     | A48   | 461:VAL   | C      | 462:THR   | N      | 1.17         |
| 1     | A48   | 560:MET   | C      | 561:ASP   | N      | 1.17         |
| 1     | N     | 163:ALA   | C      | 164:PRO   | N      | 1.16         |
| 1     | N8    | 163:ALA   | C      | 164:PRO   | N      | 1.16         |
| 1     | N16   | 163:ALA   | C      | 164:PRO   | N      | 1.16         |
| 1     | K     | 1270:VAL  | C      | 1271:GLU  | N      | 1.16         |
| 1     | K8    | 1270:VAL  | C      | 1271:GLU  | N      | 1.16         |
| 1     | C16   | 1366:GLN  | C      | 1367:ALA  | N      | 1.16         |
| 1     | C24   | 1366:GLN  | C      | 1367:ALA  | N      | 1.16         |
| 1     | W     | 588:LYS   | C      | 589:GLU   | N      | 1.16         |
| 1     | C     | 1366:GLN  | C      | 1367:ALA  | N      | 1.16         |
| 1     | C8    | 1366:GLN  | C      | 1367:ALA  | N      | 1.16         |
| 1     | C32   | 1366:GLN  | C      | 1367:ALA  | N      | 1.16         |
| 1     | R     | 1388:GLY  | C      | 1389:GLN  | N      | 1.15         |
| 1     | R8    | 1388:GLY  | C      | 1389:GLN  | N      | 1.15         |
| 1     | R16   | 1388:GLY  | C      | 1389:GLN  | N      | 1.15         |
| 1     | C16   | 1063:PRO  | C      | 1064:PHE  | N      | 1.15         |
| 1     | C24   | 1063:PRO  | C      | 1064:PHE  | N      | 1.15         |
| 1     | C     | 1063:PRO  | C      | 1064:PHE  | N      | 1.15         |
| 1     | C8    | 1063:PRO  | C      | 1064:PHE  | N      | 1.15         |
| 1     | 4     | 198:GLY   | C      | 199:THR   | N      | 1.15         |
| 1     | 48    | 198:GLY   | C      | 199:THR   | N      | 1.15         |
| 1     | C32   | 1063:PRO  | C      | 1064:PHE  | N      | 1.15         |
| 1     | C16   | 1624:LEU  | C      | 1625:SER  | N      | 1.14         |
| 1     | C24   | 1624:LEU  | C      | 1625:SER  | N      | 1.14         |
| 1     | W     | 610:PRO   | C      | 611:ALA   | N      | 1.14         |
| 1     | C     | 1624:LEU  | C      | 1625:SER  | N      | 1.14         |
| 1     | C8    | 1624:LEU  | C      | 1625:SER  | N      | 1.14         |
| 1     | C32   | 1624:LEU  | C      | 1625:SER  | N      | 1.14         |
| 1     | K     | 1051:GLU  | C      | 1052:SER  | N      | 1.12         |
| 1     | K8    | 1051:GLU  | C      | 1052:SER  | N      | 1.12         |
| 1     | V     | 832:LEU   | C      | 833:ASN   | N      | 1.11         |

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54657. These allow visual inspection of the internal detail of the map and identification of artifacts.

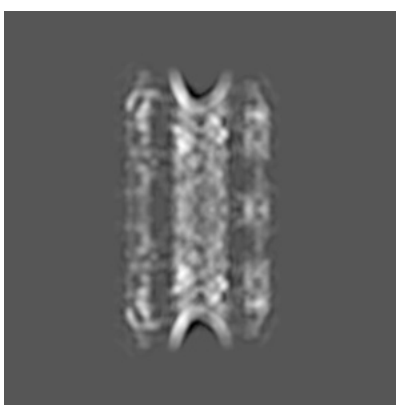
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

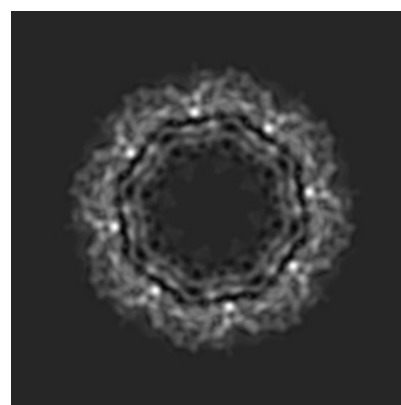
#### 6.1.1 Primary map



X



Y



Z

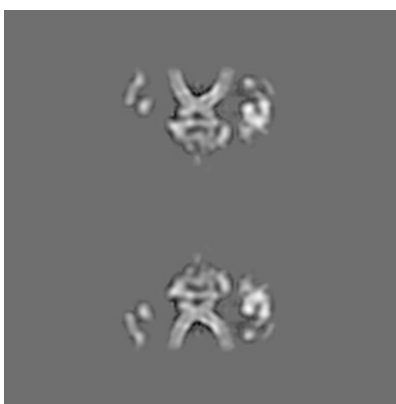
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

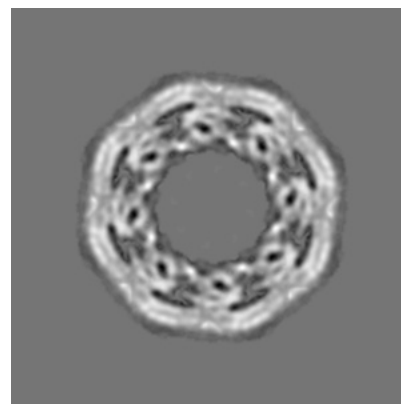
### 6.3.1 Primary map



X Index: 140



Y Index: 140

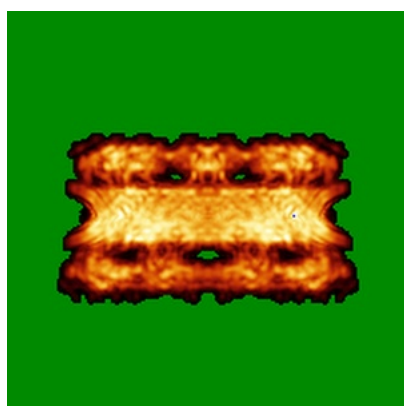


Z Index: 90

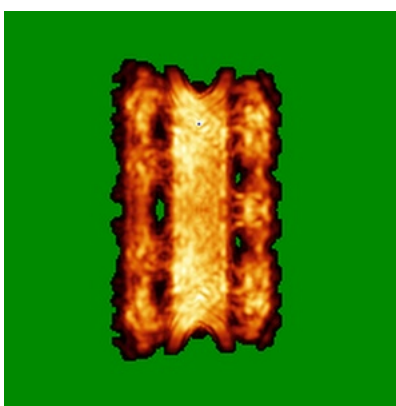
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

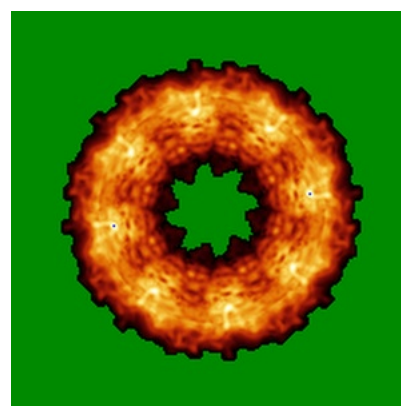
### 6.4.1 Primary map



X



Y

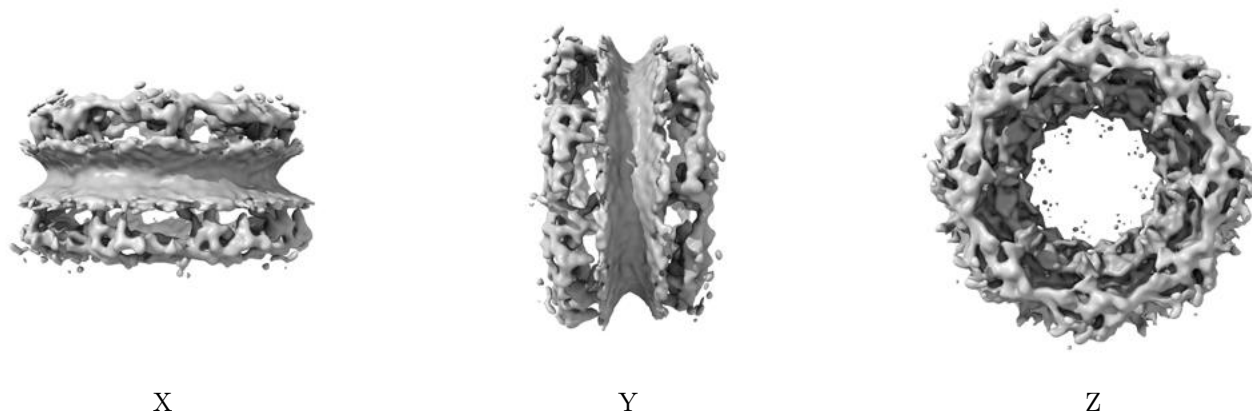


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

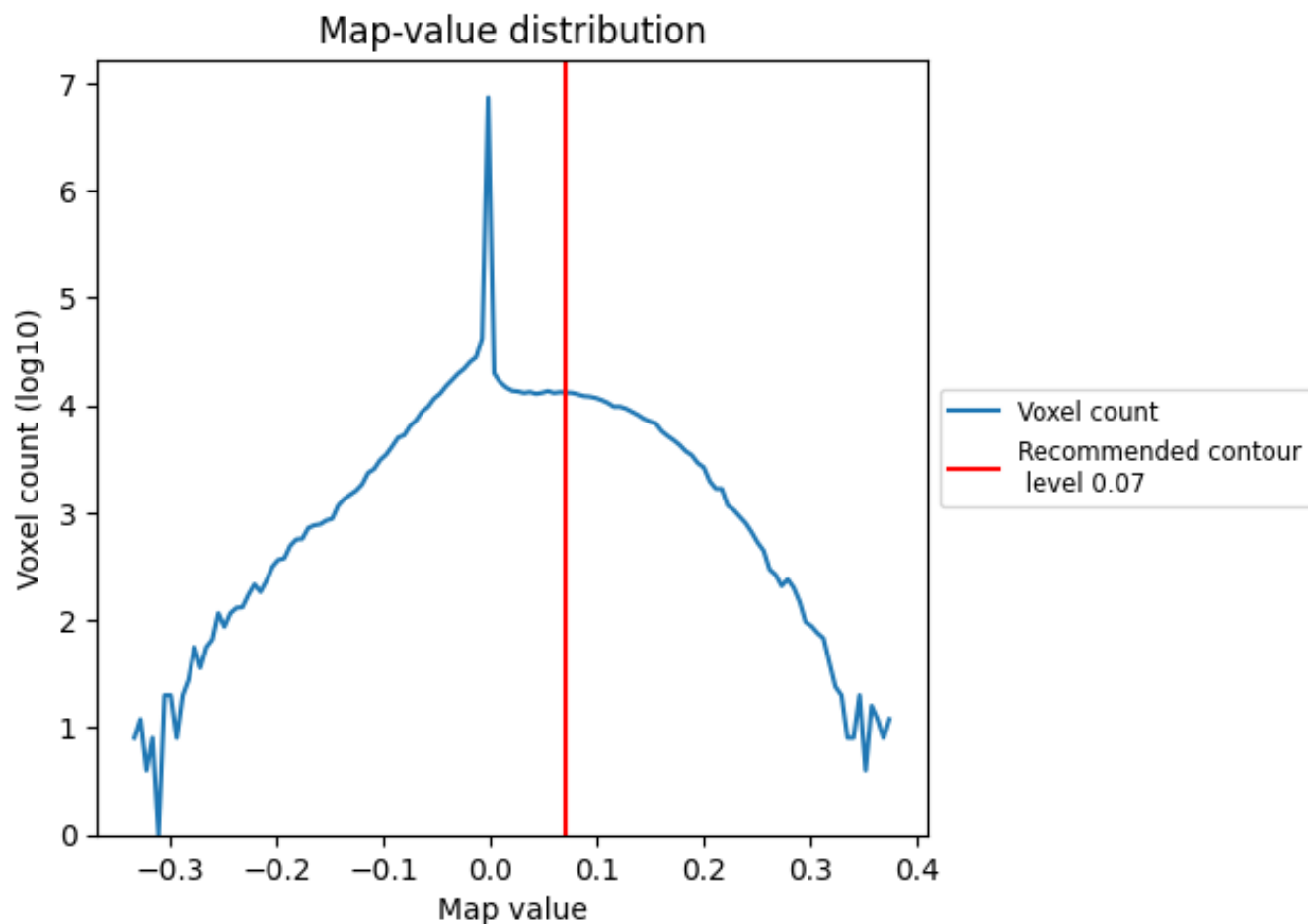
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

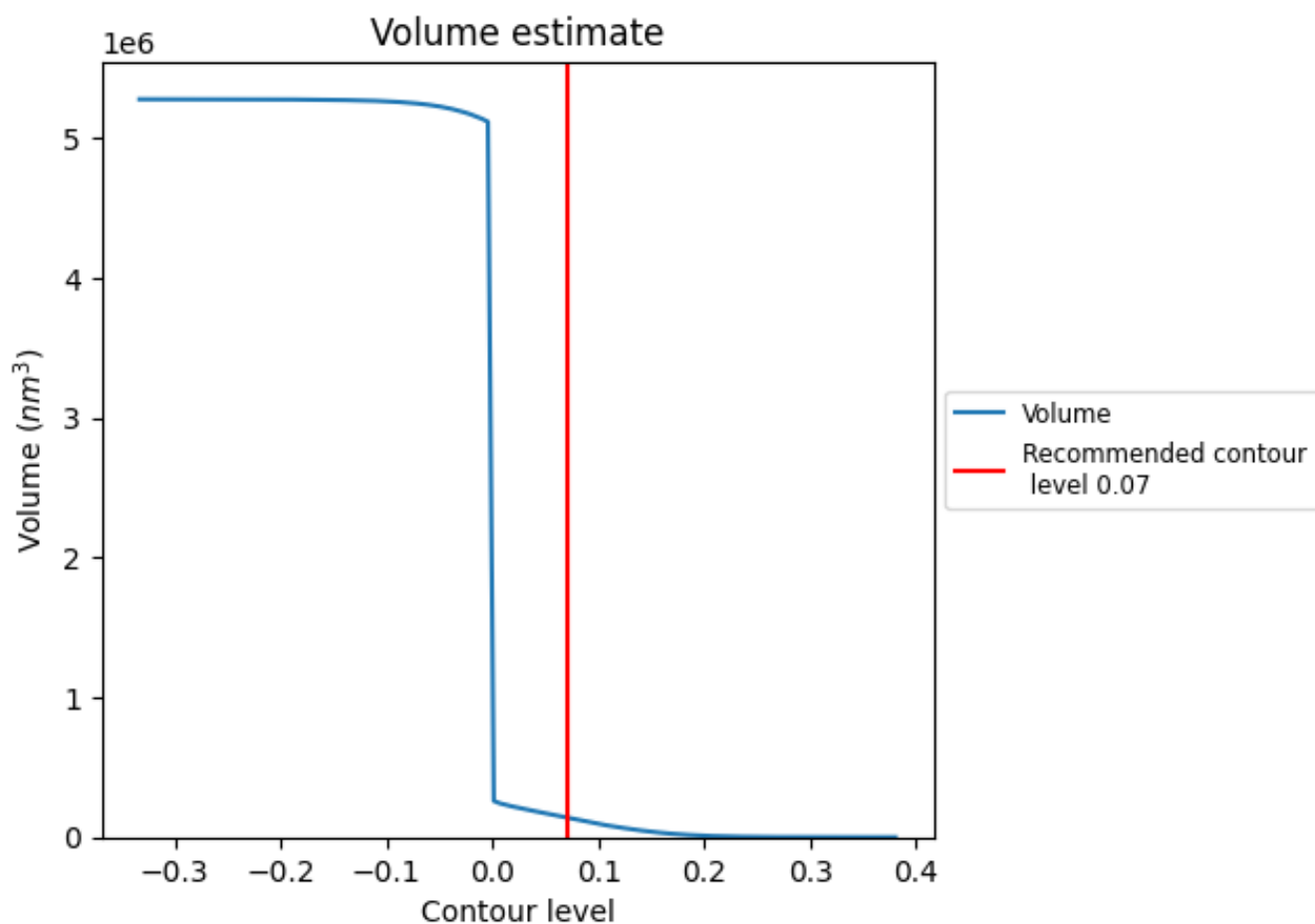
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

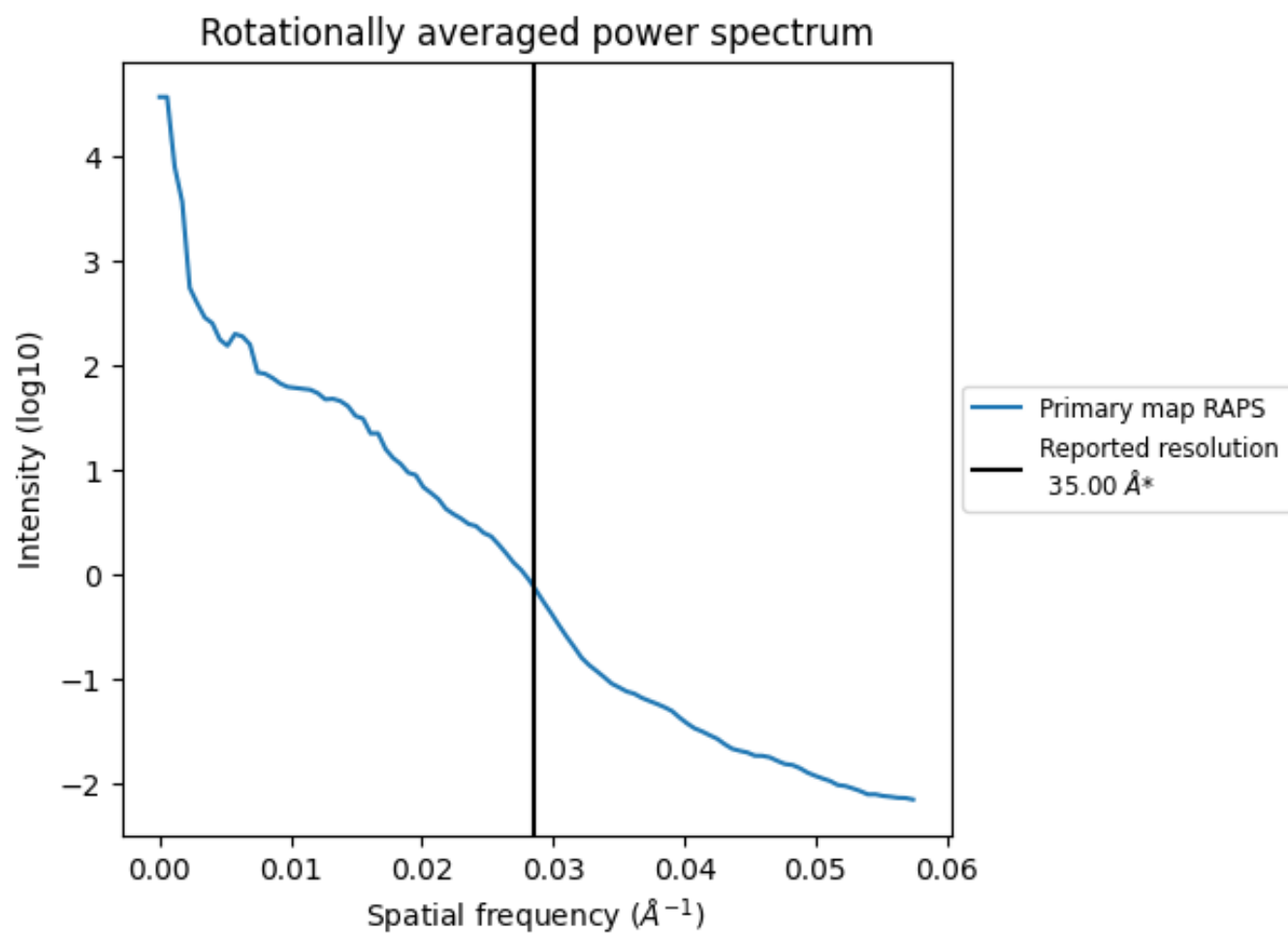
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139608  $\text{nm}^3$ ; this corresponds to an approximate mass of 126112 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.029 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

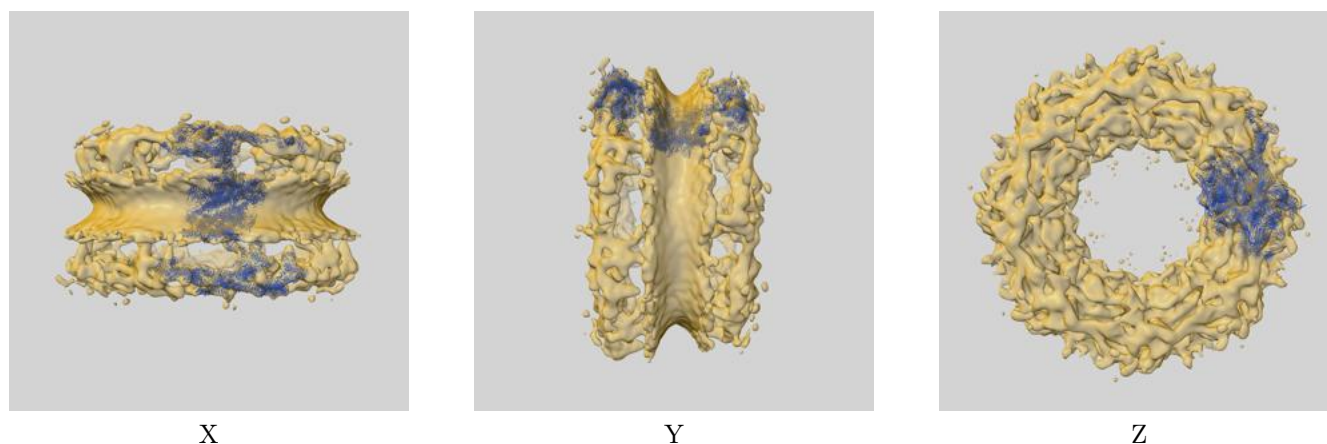
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

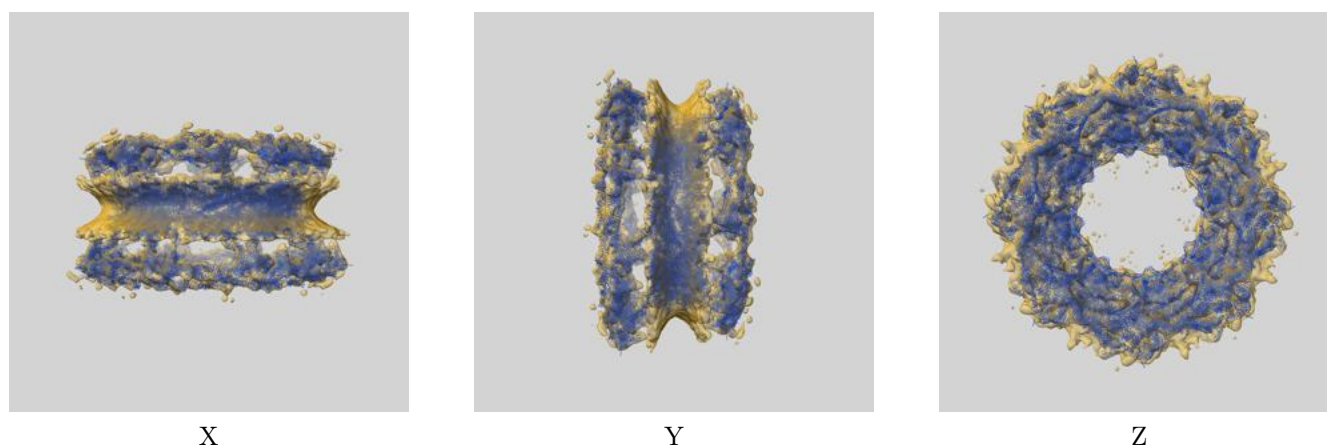
This section contains information regarding the fit between EMDB map EMD-54657 and PDB model 9SOB. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

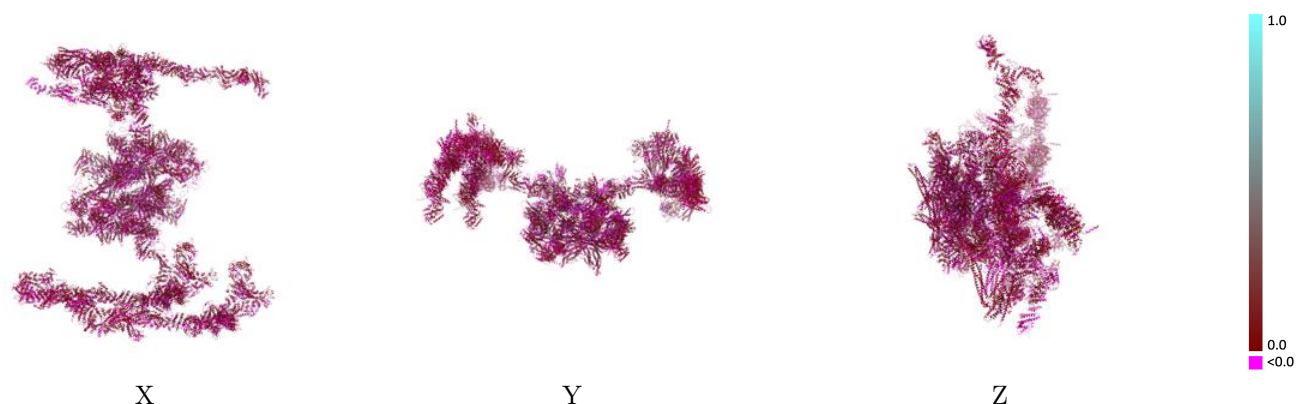


#### 9.1.2 Map-model assembly overlay [i](#)



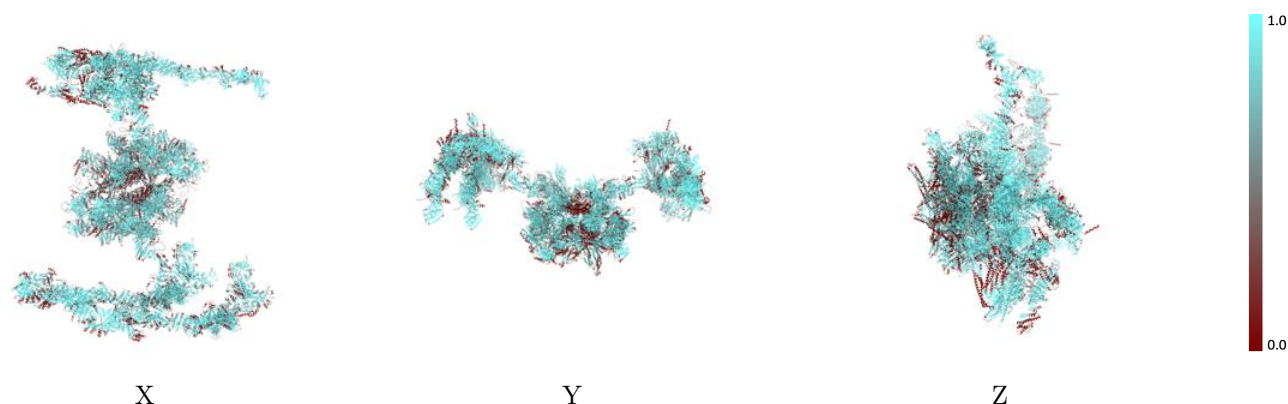
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



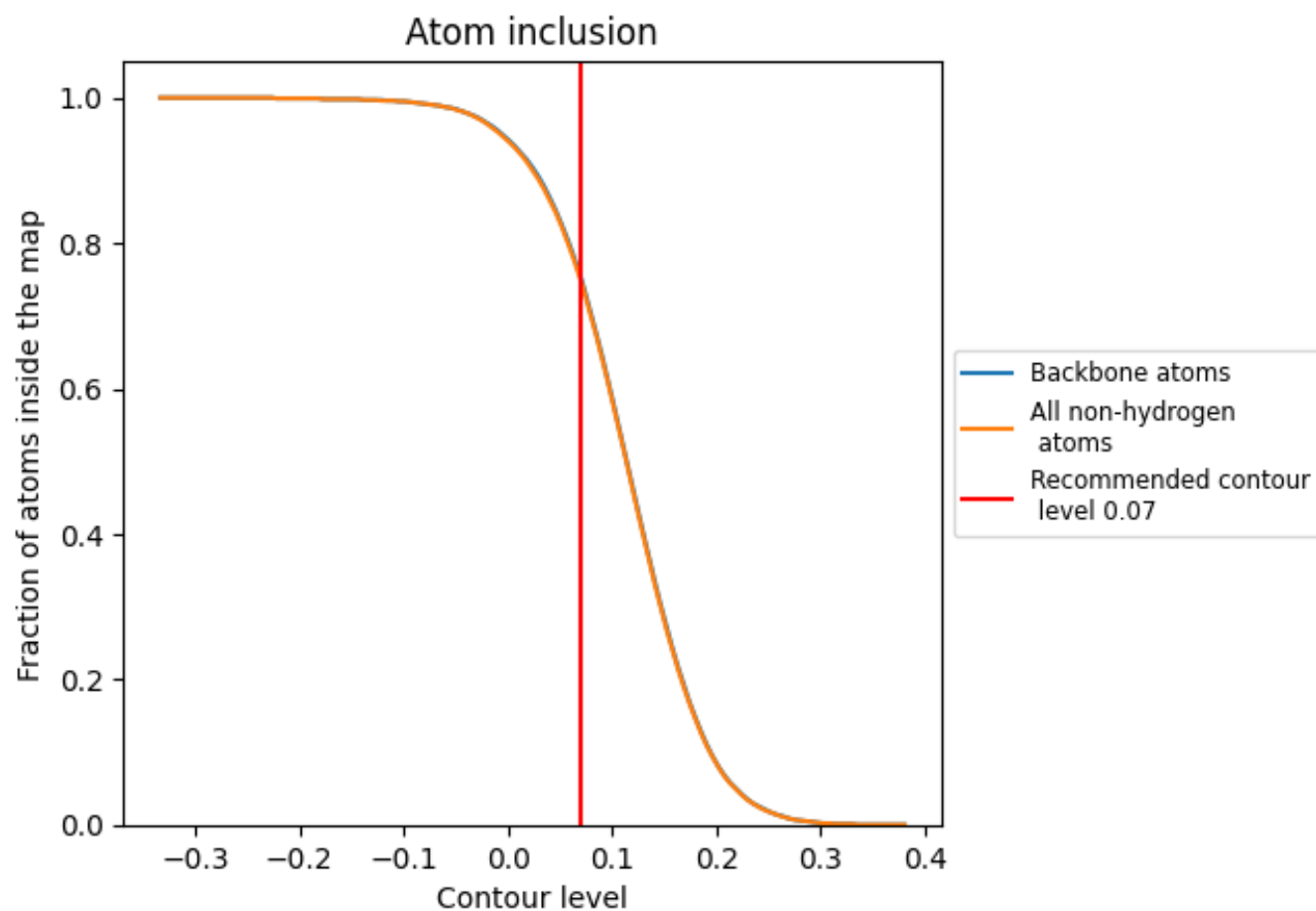
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                       |
|-------|--------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| All   |  0.7480   |  0.0350      |
| 4     |  0.8420   |  0.0370      |
| 48    |  0.8910   |  0.0370      |
| A     |  0.5230   |  0.0170      |
| A16   |  0.7680   |  0.0370      |
| A24   |  0.6180   |  0.0180      |
| A32   |  0.7450   |  0.0350      |
| A40   |  0.6230   |  0.0290      |
| A48   |  0.6960   |  0.0400      |
| A8    |  0.9810   |  0.0440      |
| B     |  0.6910   |  0.0340      |
| B8    |  0.7400   |  0.0350      |
| C     |  0.8060   |  0.0340      |
| C16   |  0.5100   |  0.0280      |
| C24   |  0.6970  |  0.0300     |
| C32   |  0.8040 |  0.0410    |
| C8    |  0.7490 |  0.0370    |
| D     |  0.7880 |  0.0320    |
| D16   |  0.7260 |  0.0290    |
| D24   |  0.7400 |  0.0260    |
| D32   |  0.7440 |  0.0330    |
| D40   |  0.7880 |  0.0360    |
| D8    |  0.6770 |  0.0300    |
| E     |  0.9250 |  0.0420    |
| E8    |  0.8990 |  0.0260    |
| F     |  0.8570 |  0.0250    |
| F16   |  0.8330 |  0.0500    |
| F24   |  0.9230 |  0.0260    |
| F8    |  0.8090 |  -0.0060 |
| H     |  0.6330 |  0.0390    |
| H16   |  0.4710 |  0.0260    |
| H24   |  0.6750 |  0.0350    |
| H8    |  0.3240 |  0.0310    |
| I     |  0.5440 |  0.0370    |
| I16   |  0.5770 |  0.0310    |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| I24   |  0.6450   |  0.0470   |
| I8    |  0.4490   |  0.0230   |
| J     |  0.4350   |  0.0320   |
| J16   |  0.7560   |  0.0700   |
| J24   |  0.7140   |  0.0420   |
| J32   |  0.6230   |  0.0560   |
| J8    |  0.6470   |  0.0580   |
| K     |  0.7940   |  0.0400   |
| K16   |  0.8170   |  0.0520   |
| K8    |  0.6200   |  0.0310   |
| L     |  0.8160   |  0.0450   |
| L16   |  0.7840   |  0.0370   |
| L8    |  0.8380   |  0.0370   |
| M     |  0.8920   |  0.0450   |
| M16   |  0.7960   |  0.0360   |
| M8    |  0.7930   |  0.0400   |
| N     |  0.9880   |  0.0350   |
| N16   |  0.8080   |  0.0320   |
| N8    |  0.8520   |  0.0260   |
| O     |  0.9760  |  0.0380  |
| O16   |  0.9240 |  0.0430 |
| O8    |  0.9770 |  0.0460 |
| P     |  0.8200 |  0.0340 |
| P16   |  0.8000 |  0.0410 |
| P8    |  0.8740 |  0.0440 |
| Q     |  0.8400 |  0.0300 |
| Q16   |  0.7150 |  0.0410 |
| Q8    |  0.8080 |  0.0370 |
| R     |  0.8590 |  0.0300 |
| R16   |  0.7130 |  0.0360 |
| R8    |  0.8030 |  0.0380 |
| T     |  0.8390 |  0.0470 |
| T16   |  0.6860 |  0.0300 |
| T8    |  0.8460 |  0.0400 |
| V     |  0.5360 |  0.0540 |
| W     |  0.7110 |  0.0310 |