



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:34 PM UTC

PDB ID : 7DKF / pdb\_00007dkf  
EMDB ID : EMD-30706  
Title : Activity optimized supercomplex state4  
Authors : Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.  
Deposited on : 2020-11-24  
Resolution : 8.30 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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

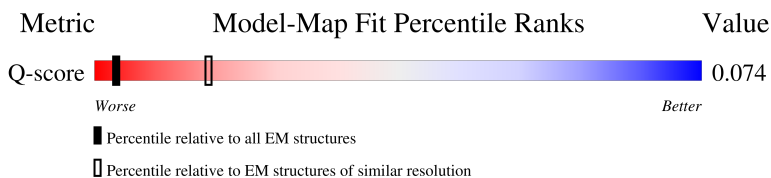
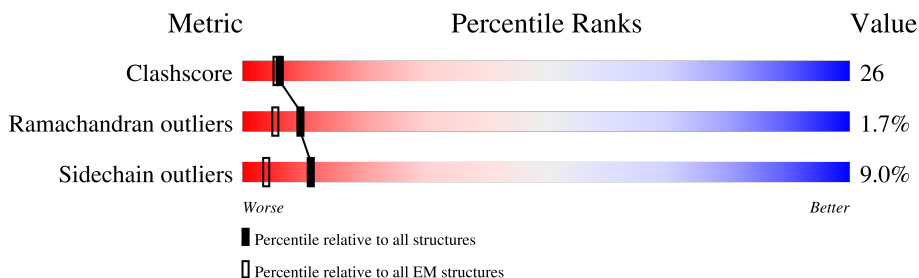
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.30 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                       | 280 ( 7.82 - 8.80 )                                      |

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   | A1    | 480    |                  |
| 1   | M1    | 480    |                  |
| 2   | B1    | 453    |                  |
| 2   | N1    | 453    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C1    | 379    |                  |
| 3   | O1    | 379    |                  |
| 4   | D1    | 325    |                  |
| 4   | P1    | 325    |                  |
| 5   | E1    | 196    |                  |
| 5   | Q1    | 196    |                  |
| 6   | F1    | 111    |                  |
| 6   | R1    | 111    |                  |
| 7   | G1    | 82     |                  |
| 7   | S1    | 82     |                  |
| 8   | H1    | 91     |                  |
| 8   | T1    | 91     |                  |
| 9   | I1    | 78     |                  |
| 9   | U1    | 78     |                  |
| 10  | J1    | 64     |                  |
| 10  | V1    | 64     |                  |
| 11  | K1    | 56     |                  |
| 11  | W1    | 56     |                  |
| 12  | 22    | 347    |                  |
| 13  | 32    | 115    |                  |
| 14  | 42    | 459    |                  |
| 15  | 52    | 98     |                  |
| 16  | 72    | 175    |                  |
| 17  | 82    | 444    |                  |
| 18  | 92    | 217    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 19  | A2    | 704    |                  |
| 20  | B2    | 430    |                  |
| 21  | C2    | 228    |                  |
| 22  | D2    | 179    |                  |
| 23  | E2    | 176    |                  |
| 24  | F2    | 75     |                  |
| 25  | G2    | 133    |                  |
| 26  | H2    | 105    |                  |
| 27  | I2    | 96     |                  |
| 28  | J2    | 70     |                  |
| 29  | K2    | 98     |                  |
| 30  | L2    | 83     |                  |
| 31  | N2    | 115    |                  |
| 32  | O2    | 127    |                  |
| 33  | P2    | 112    |                  |
| 34  | Q2    | 171    |                  |
| 35  | R2    | 345    |                  |
| 36  | S2    | 320    |                  |
| 37  | T2    | 140    |                  |
| 38  | U2    | 145    |                  |
| 39  | V2    | 143    |                  |
| 40  | M2    | 88     |                  |
| 40  | W2    | 88     |                  |
| 41  | X2    | 57     |                  |
| 42  | Y2    | 72     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 43  | Z2    | 97     |                  |
| 44  | a2    | 128    |                  |
| 45  | b2    | 143    |                  |
| 46  | c2    | 127    |                  |
| 47  | d2    | 136    |                  |
| 48  | f2    | 178    |                  |
| 49  | h2    | 125    |                  |
| 50  | i2    | 49     |                  |
| 51  | j2    | 120    |                  |
| 52  | 12    | 318    |                  |
| 53  | 62    | 606    |                  |
| 54  | g2    | 176    |                  |
| 55  | e2    | 158    |                  |
| 56  | A3    | 514    |                  |
| 57  | B3    | 227    |                  |
| 58  | C3    | 261    |                  |
| 59  | D3    | 169    |                  |
| 60  | E3    | 152    |                  |
| 61  | F3    | 129    |                  |
| 62  | G3    | 97     |                  |
| 63  | H3    | 86     |                  |
| 64  | I3    | 74     |                  |
| 65  | J3    | 80     |                  |
| 66  | K3    | 80     |                  |
| 67  | L3    | 63     |                  |

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| Mol | Chain | Length | Quality of chain       |
|-----|-------|--------|------------------------|
| 68  | M3    | 70     | <p>24% 43% 17% 39%</p> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 75  | SF4  | A2    | 801 | -         | -        | X       | -                |
| 75  | SF4  | A2    | 802 | -         | -        | X       | -                |

## 2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 105456 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A1    | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3356  | 2098 | 595 | 643 | 20 |         |       |
| 1   | M1    | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3356  | 2098 | 595 | 643 | 20 |         |       |

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B1    | 419      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3141  | 1972 | 556 | 606 | 7 |         |       |
| 2   | N1    | 419      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3141  | 1972 | 556 | 606 | 7 |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C1    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3011  | 2018 | 472 | 502 | 19 |         |       |
| 3   | O1    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3011  | 2018 | 472 | 502 | 19 |         |       |

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D1    | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1919  | 1225 | 330 | 349 | 15 |         |       |
| 4   | P1    | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1919  | 1225 | 330 | 349 | 15 |         |       |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E1    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 566   | 352 | 94  | 118 | 2 |         |       |
| 5   | Q1    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 263 | 291 | 8 |         |       |

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F1    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 579 | 167 | 168 | 2 |         |       |
| 6   | R1    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 579 | 167 | 168 | 2 |         |       |

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G1    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 682   | 441 | 128 | 112 | 1 |         |       |
| 7   | S1    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 682   | 441 | 128 | 112 | 1 |         |       |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 8   | H1    | 64       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 524   | 316 | 96 | 107 | 5 |         |       |
| 8   | T1    | 64       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 524   | 316 | 96 | 107 | 5 |         |       |

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | I1    | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 248   | 152 | 51 | 44 | 1 |         |       |
| 9   | U1    | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 248   | 152 | 51 | 44 | 1 |         |       |

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | J1    | 62       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 511   | 335 | 89 | 87 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | V1    | 62       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 511   | 335 | 89 | 87 |         |       |

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | K1    | 22       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 164   | 109 | 29 | 26 |         |       |
| 11  | W1    | 22       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 164   | 109 | 29 | 26 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | 22    | 344      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2582  | 1707 | 404 | 437 | 34 |         |       |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | 32    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 719   | 492 | 104 | 120 | 3 |         |       |

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | 42    | 458      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3447  | 2293 | 548 | 574 | 32 |         |       |

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | 52    | 96       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 697   | 454 | 109 | 124 | 10 |         |       |

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | 72    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1186  | 798 | 179 | 202 | 7 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | 82    | 427      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2965  | 1864 | 552 | 534 | 15 |         |       |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | 92    | 207      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1535  | 978 | 261 | 286 | 10 |         |       |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | A2    | 688      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5183  | 3254 | 915 | 978 | 36 |         |       |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | B2    | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3076  | 1963 | 530 | 559 | 24 |         |       |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | C2    | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1102 | 294 | 306 | 3 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | D2    | 152      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1200  | 769 | 209 | 208 | 14 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | E2    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1388  | 874 | 239 | 264 | 11 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 24  | F2    | 28       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 183   | 116 | 32 | 35 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | G2    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 619 | 177 | 182 | 3 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | H2    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 494 | 147 | 134 | 5 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | I2    | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 532   | 332 | 99 | 98 | 3 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | J2    | 69       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 530   | 344 | 96 | 88 | 2 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 29  | K2    | 84       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 652   | 409 | 125 | 118 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 30  | L2    | 80       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 602   | 398 | 97 | 105 | 2 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | N2    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 559 | 149 | 152 | 2 |         |       |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | O2    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 925   | 595 | 170 | 156 | 4 |         |       |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | P2    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 442 | 128 | 126 | 2 |         |       |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Q2    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1345  | 851 | 242 | 243 | 9 |         |       |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | R2    | 306      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2334  | 1505 | 417 | 409 | 3 |         |       |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | S2    | 319      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2299  | 1457 | 395 | 438 | 9 |         |       |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | T2    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 599 | 165 | 172 | 6 |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | U2    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 480 | 123 | 128 | 3 |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | V2    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 702 | 189 | 193 | 9 |         |       |

- Molecule 40 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 40  | W2    | 83       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 596   | 386 | 95 | 111 | 4 |         |       |
| 40  | M2    | 80       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 642   | 413 | 96 | 128 | 5 |         |       |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 41  | X2    | 49       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 372   | 243 | 64 | 65 |         |       |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | Y2    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 409   | 277 | 65 | 66 | 1 |         |       |

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | Z2    | 74       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 493   | 320 | 89 | 82 | 2 |         |       |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | a2    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 550 | 159 | 148 |   |         |       |

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | b2    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 672 | 190 | 168 | 2 |         |       |

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | c2    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 391 | 119 | 107 |   |         |       |

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | d2    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 134 | 125 | 4 |         |       |

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | f2    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 739 | 205 | 208 | 4 |         |       |

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | h2    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 721   | 461 | 123 | 135 | 2 |         |       |

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 50  | i2    | 38       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 277   | 185 | 46 | 46 |         |       |

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | j2    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 892   | 587 | 149 | 153 | 3 |         |       |

- Molecule 52 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | 12    | 309      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2442  | 1642 | 376 | 401 | 23 |         |       |

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | 62    | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4765  | 3172 | 732 | 819 | 42 |         |       |

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | g2    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1351  | 849 | 246 | 248 | 8 |         |       |

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | e2    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 864   | 539 | 161 | 160 | 4 |         |       |

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | A3    | 514      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4025  | 2690 | 623 | 677 | 35 |         |       |

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 57  | B3    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1822  | 1184 | 281 | 339 | 18 |         |       |

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | C3    | 261      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2124  | 1420 | 338 | 353 | 13 |         |       |

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | D3    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1195  | 777 | 196 | 218 | 4 |         |       |

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | E3    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 878   | 558 | 150 | 168 | 2 |         |       |

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | F3    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 464 | 134 | 145 | 5 |         |       |

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | G3    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 431 | 129 | 110 | 1 |         |       |

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | H3    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 628   | 395 | 114 | 114 | 5 |         |       |

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 64  | I3    | 73       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 598   | 388 | 107 | 99 | 4 |         |       |

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 65  | J3    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 441   | 285 | 73 | 80 | 3 |         |       |

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 66  | K3    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 384   | 250 | 65 | 67 | 2 |         |       |

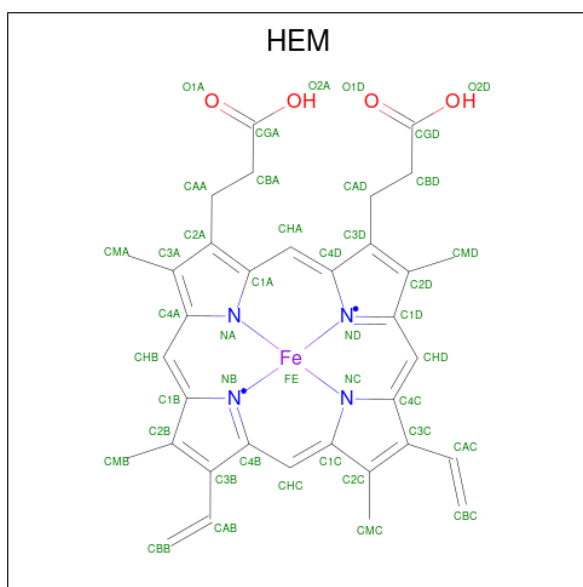
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 67  | L3    | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 386   | 257 | 65 | 62 | 2 |         |       |

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

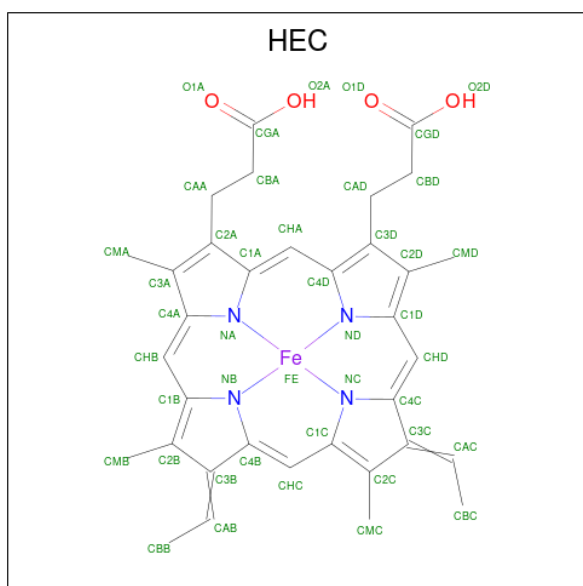
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 68  | M3    | 43       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |       |

- Molecule 69 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



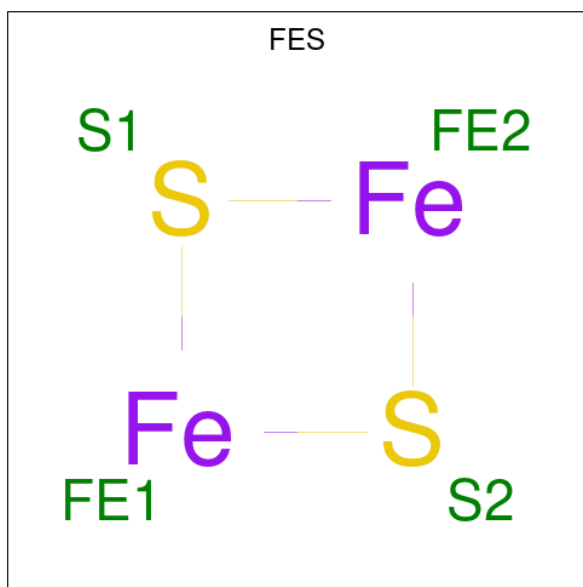
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 69  | C1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 69  | C1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 69  | O1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 69  | O1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 70 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



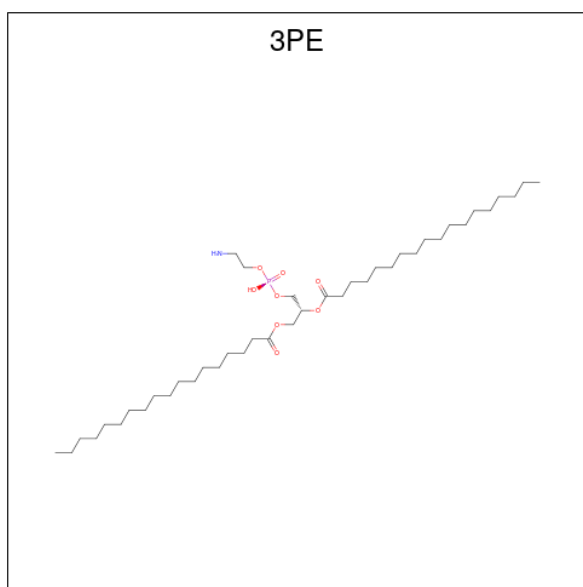
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 70  | D1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 70  | P1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



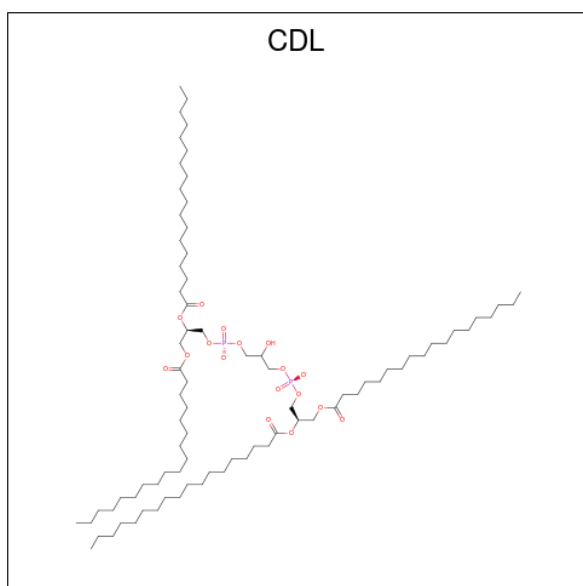
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 71  | Q1    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 71  | 92    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 71  | A2    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



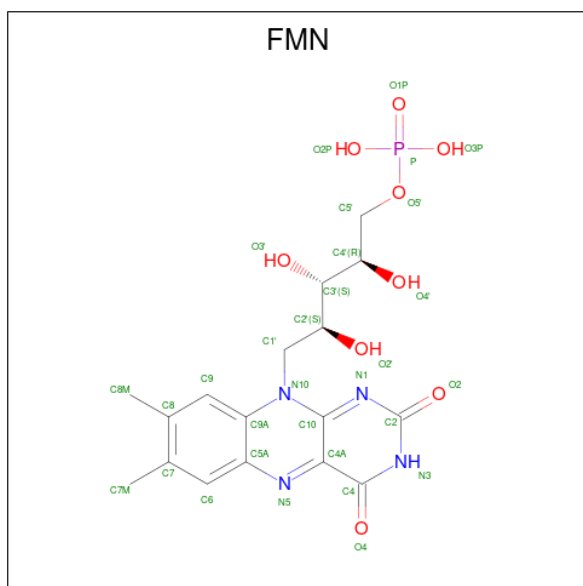
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 72  | 22    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 72  | 42    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 72  | B2    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |

- Molecule 73 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 73  | 42    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 82    | 63 | 17 | 2 |         |

- Molecule 74 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).

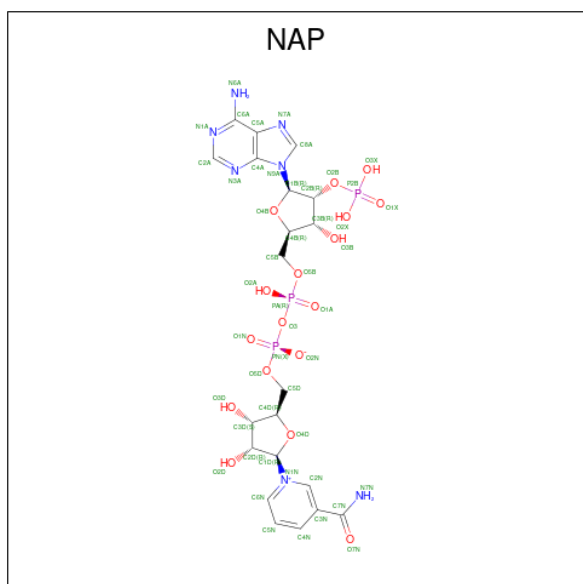


| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 75  | 82    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 75  | A2    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 75  | A2    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 75  | D2    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 75  | E2    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 75  | E2    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |

- Molecule 76 is ZINC ION (CCD ID: ZN) (formula: Zn).

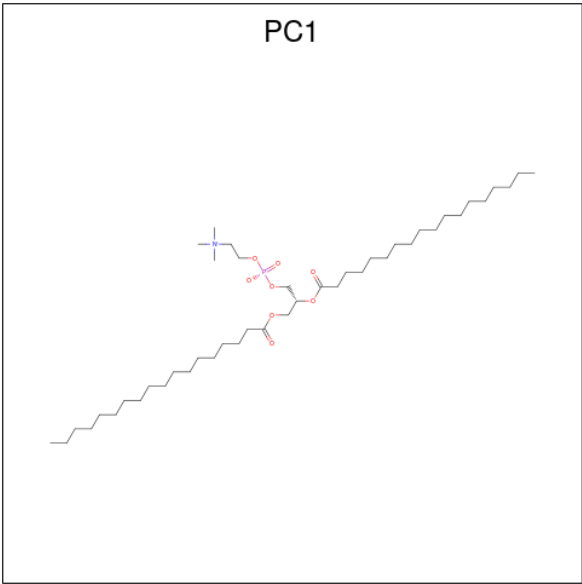
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 76  | I2    | 1        | Total Zn<br>1 1 | 0       |
| 76  | F3    | 1        | Total Zn<br>1 1 | 0       |

- Molecule 77 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



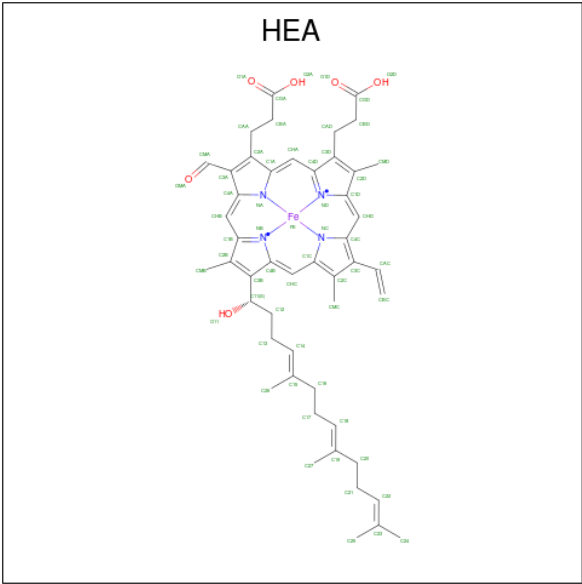
| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 77  | R2    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |

- Molecule 78 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 78  | S2    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 78  | j2    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 79  | A3    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |
| 79  | A3    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |

- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 80  | A3    | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |
| 80  | B3    | 2        | Total | Cu | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

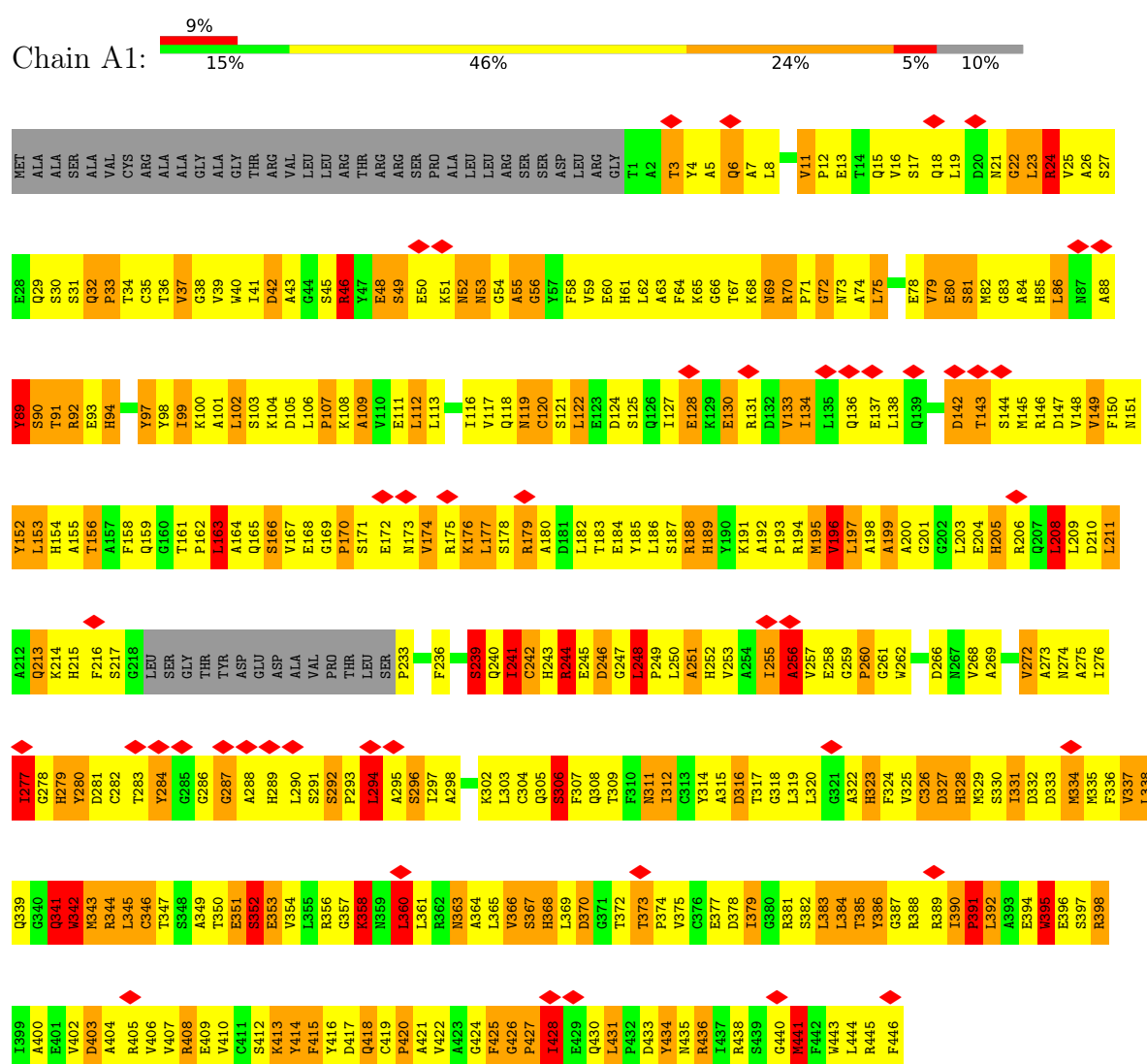
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 81  | A3    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |



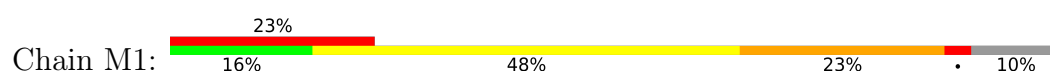
### 3 Residue-property plots

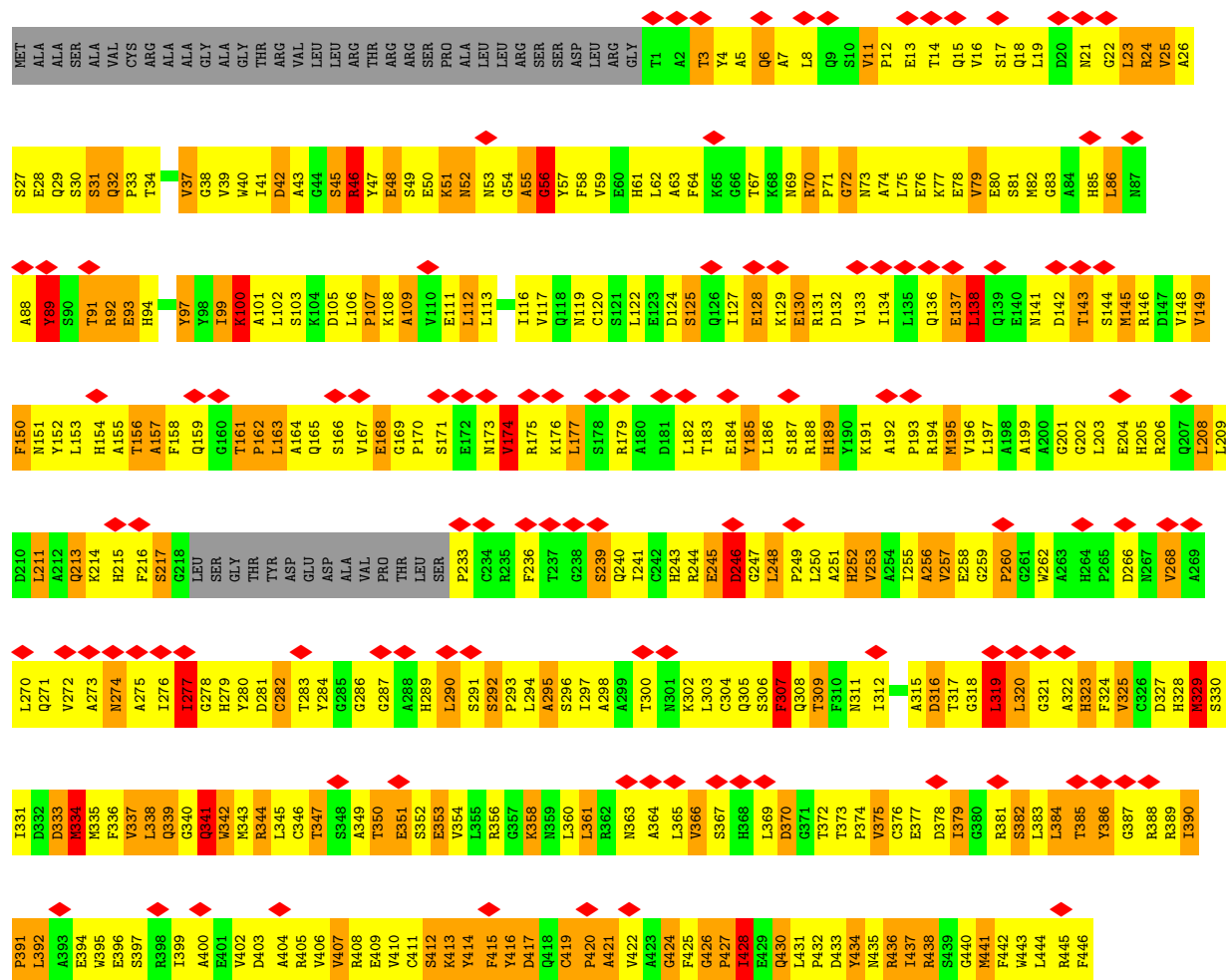
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytochrome b-c1 complex subunit 1, mitochondrial

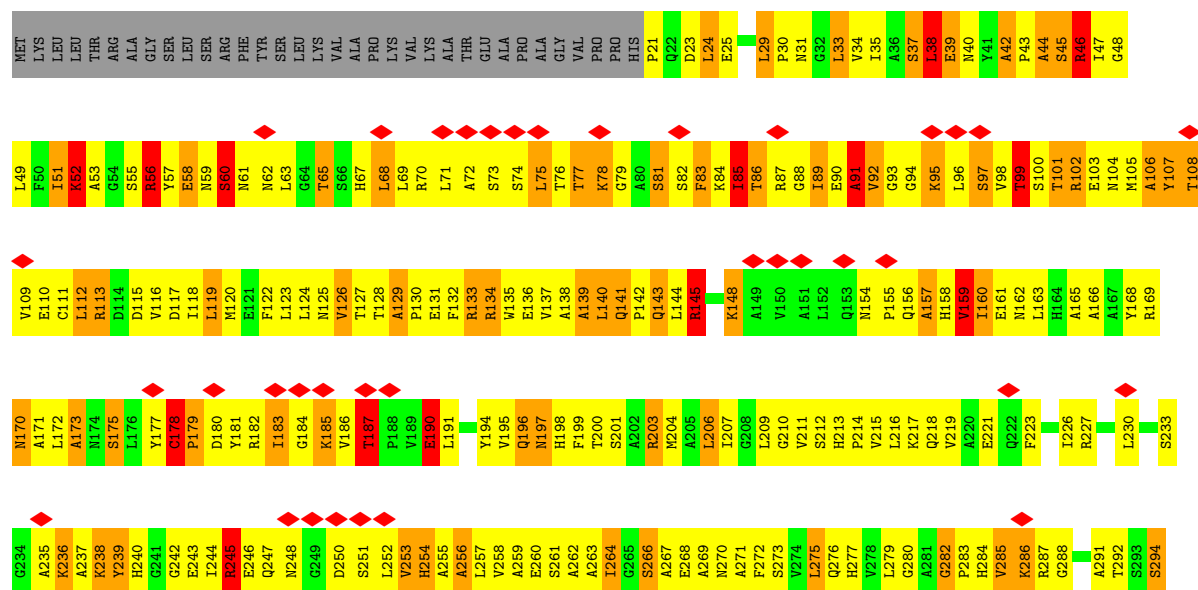
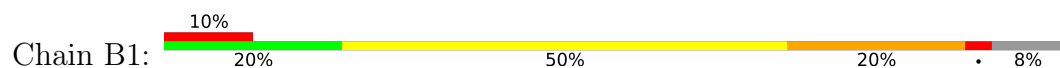


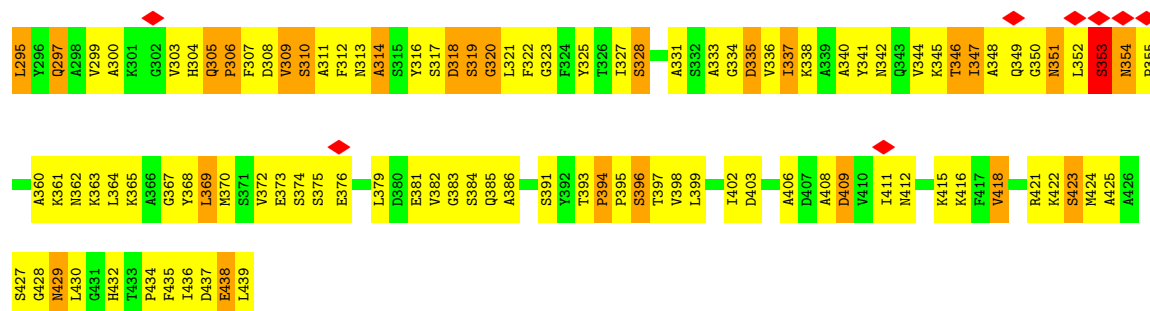
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



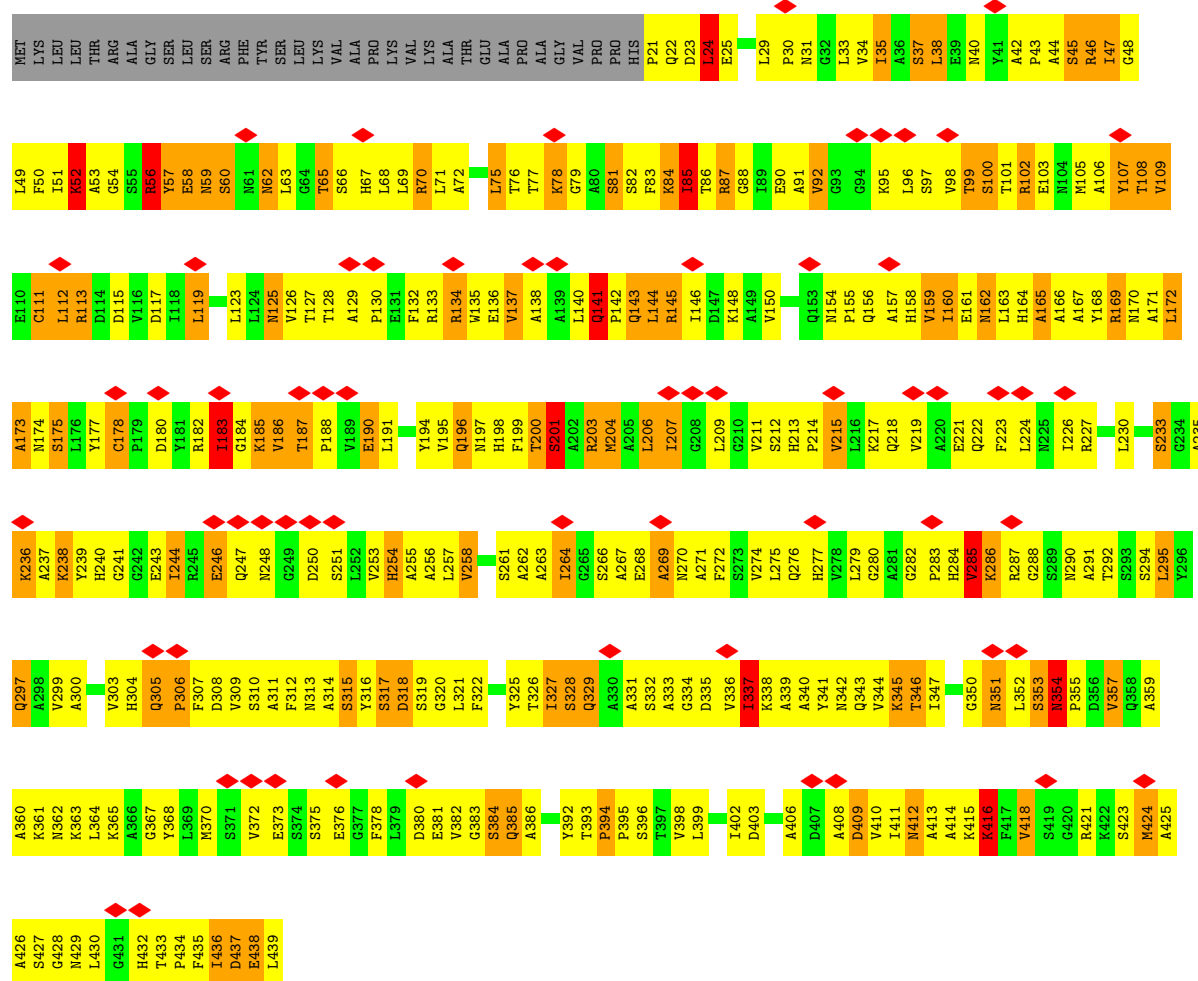
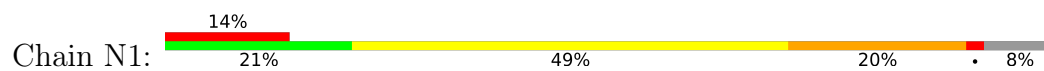


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

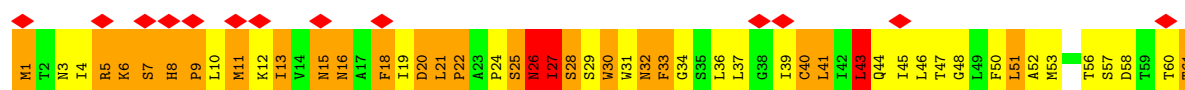
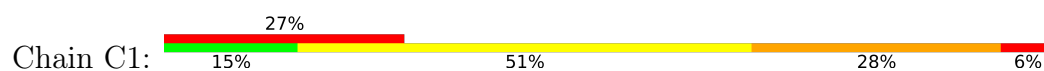


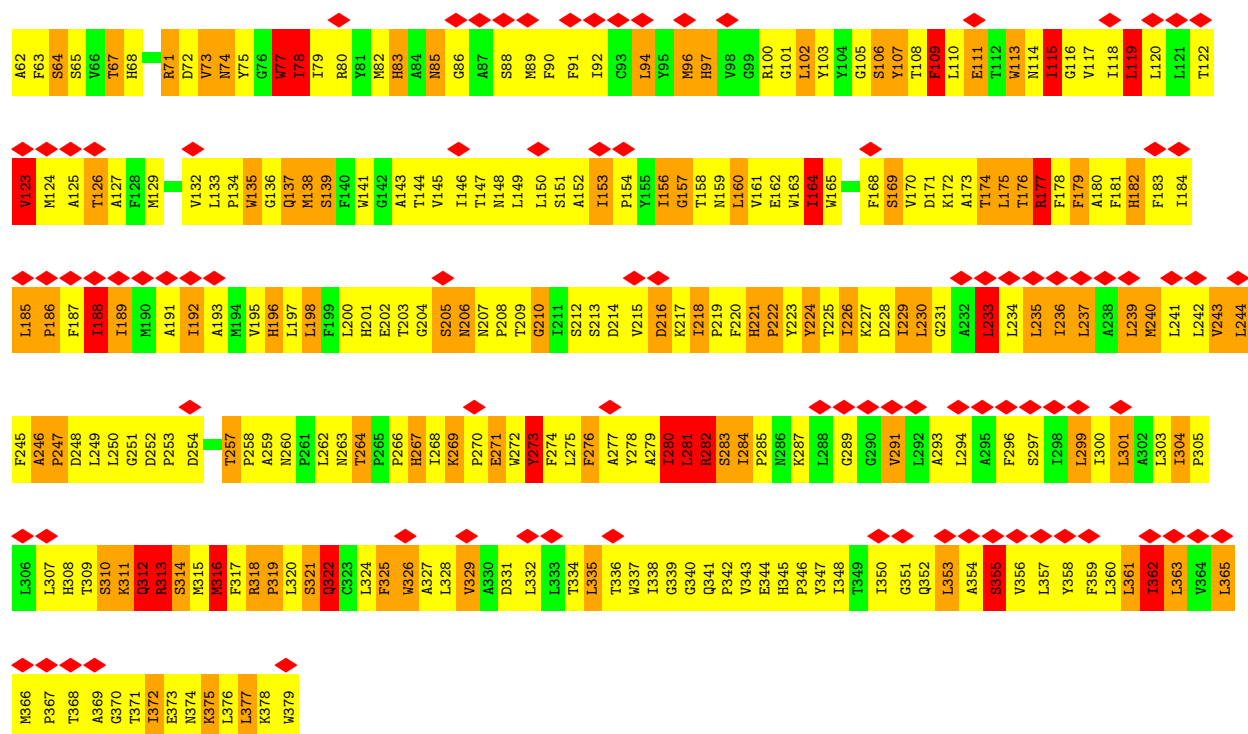


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

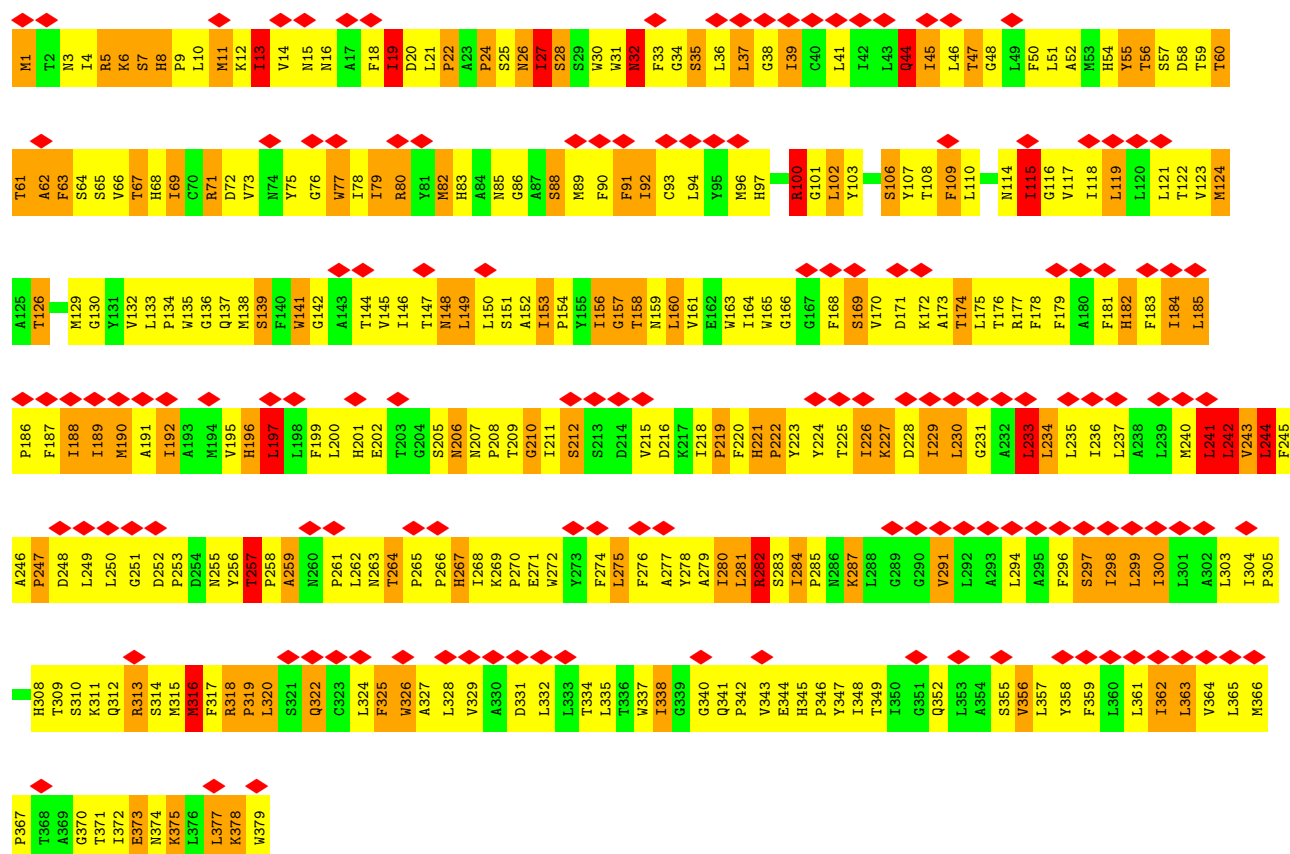
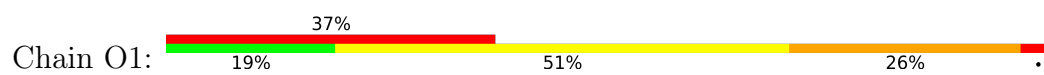


• Molecule 3: Cytochrome b

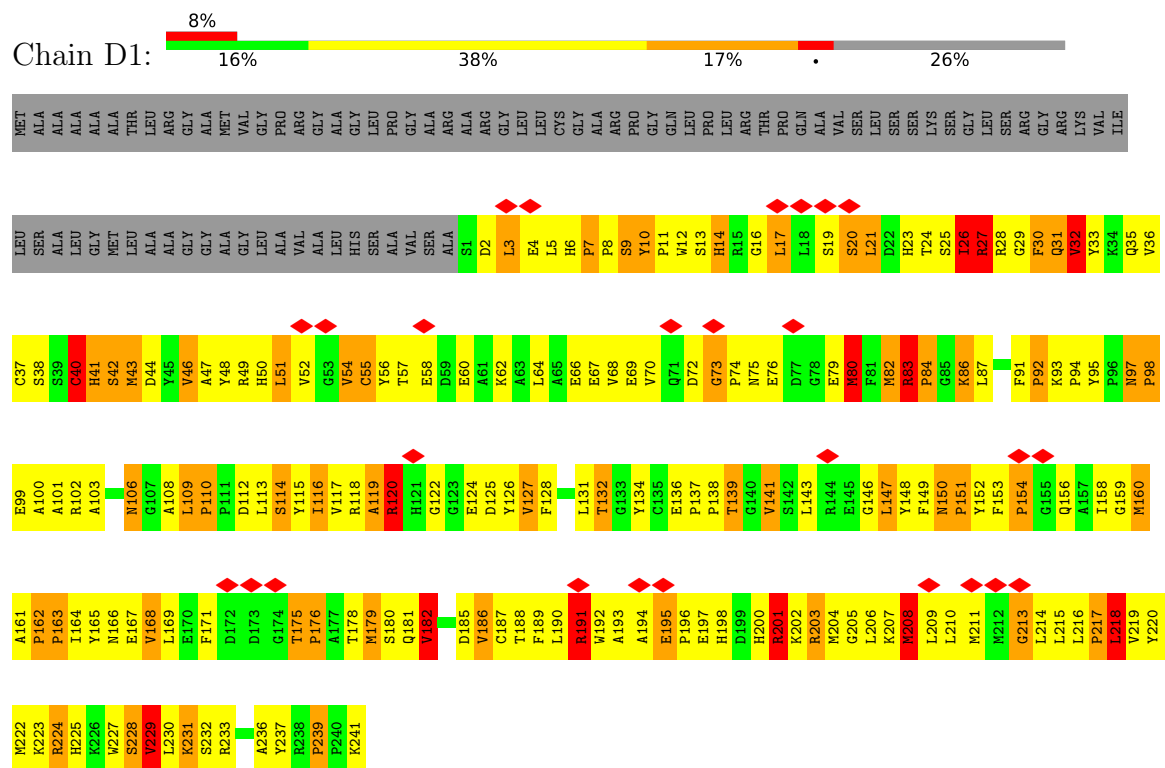




### • Molecule 3: Cytochrome b



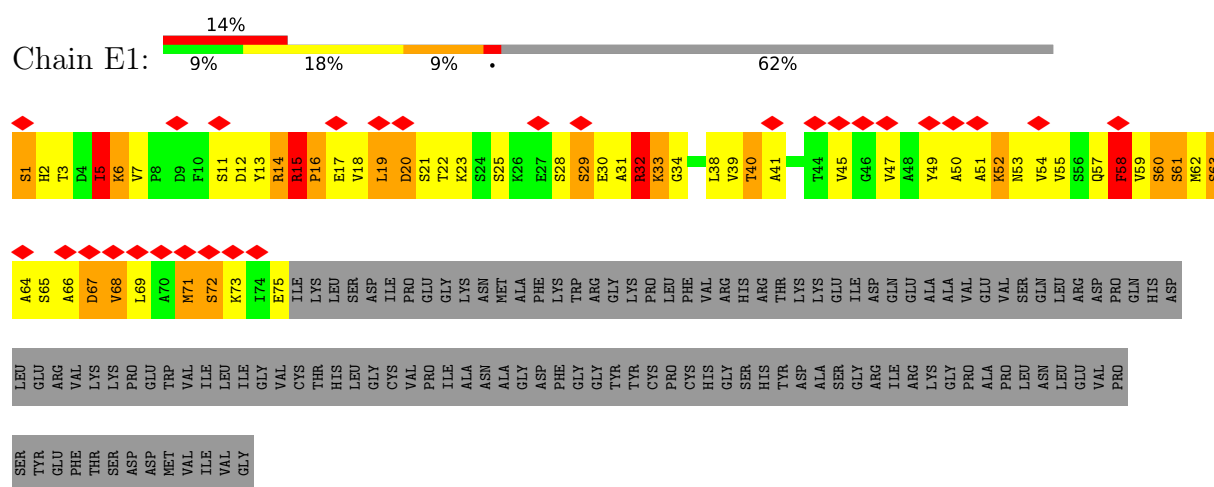
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



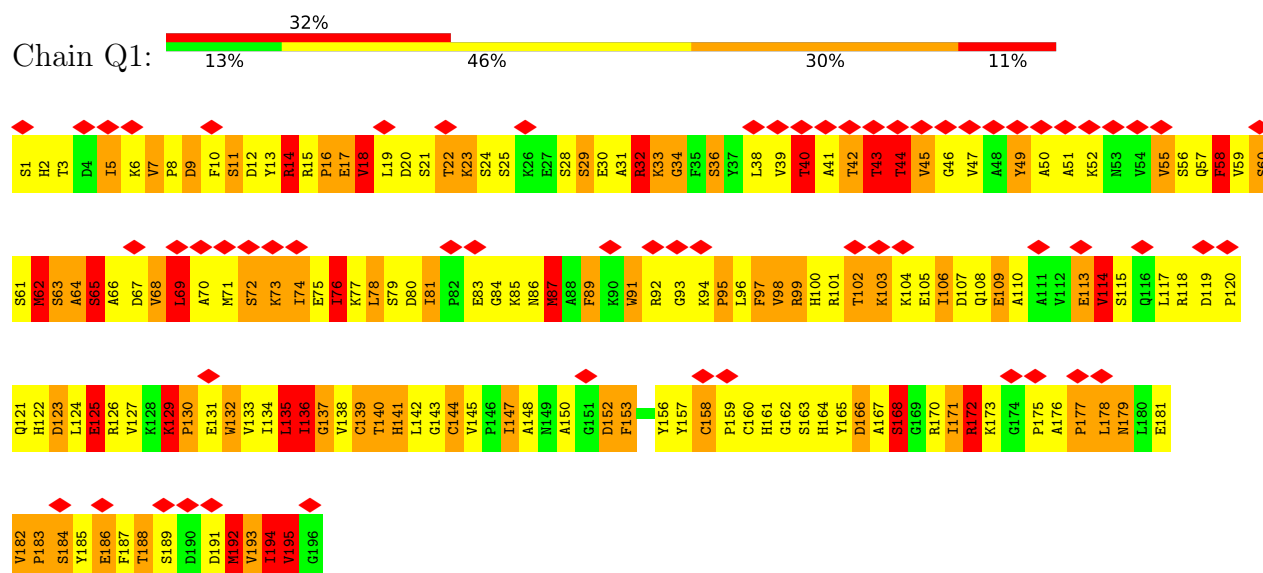
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



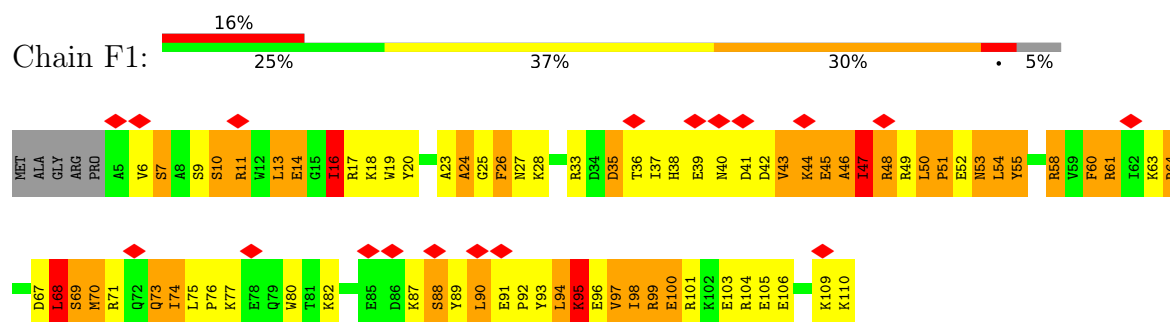
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



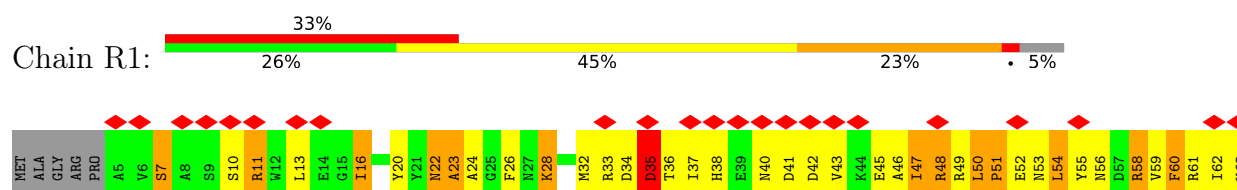
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

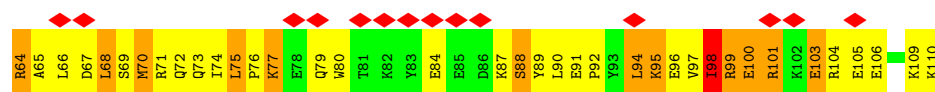


• Molecule 6: Cytochrome b-c1 complex subunit 7

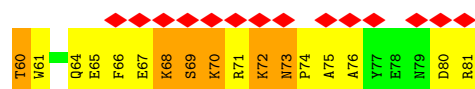
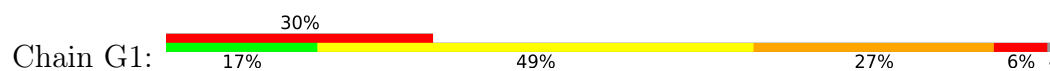


• Molecule 6: Cytochrome b-c1 complex subunit 7

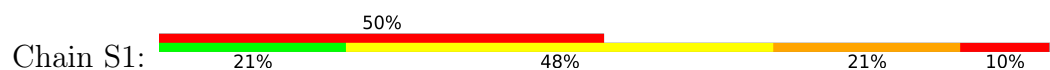




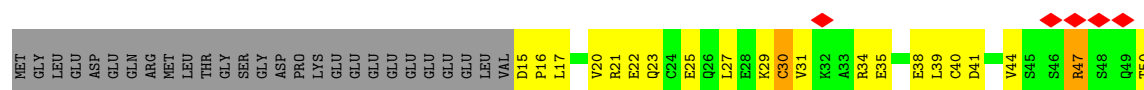
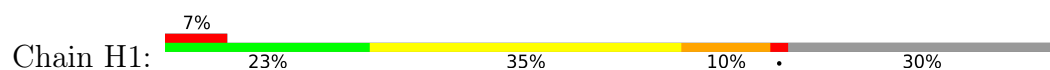
• Molecule 7: Cytochrome b-c1 complex subunit 8



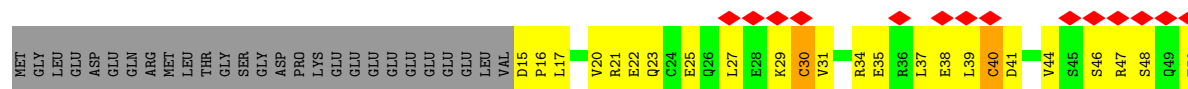
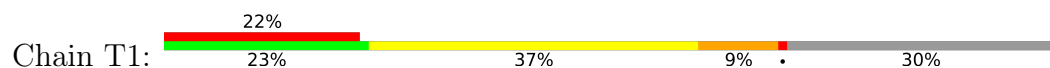
• Molecule 7: Cytochrome b-c1 complex subunit 8



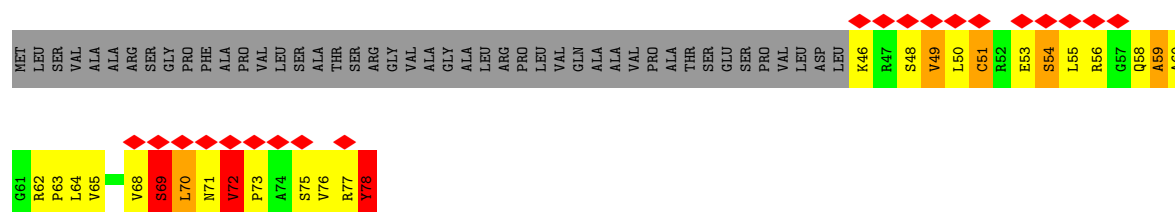
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



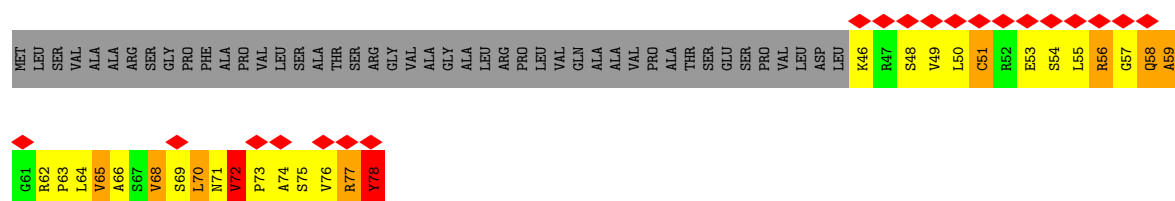
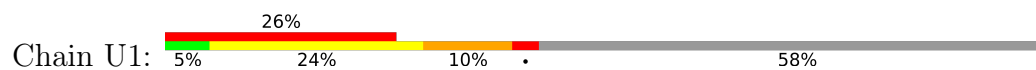
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



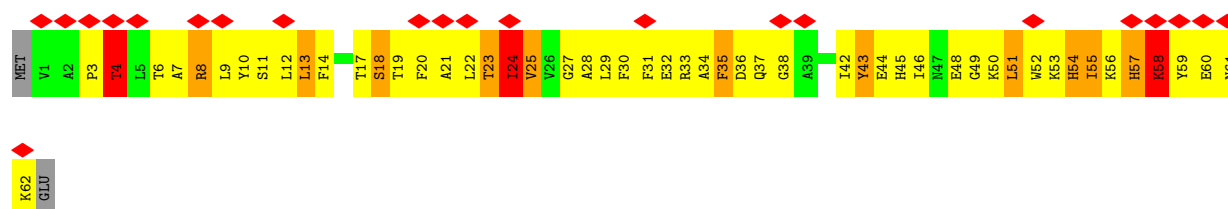
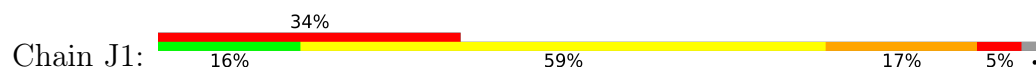
• Molecule 9: Cytochrome b-c1 complex subunit 9



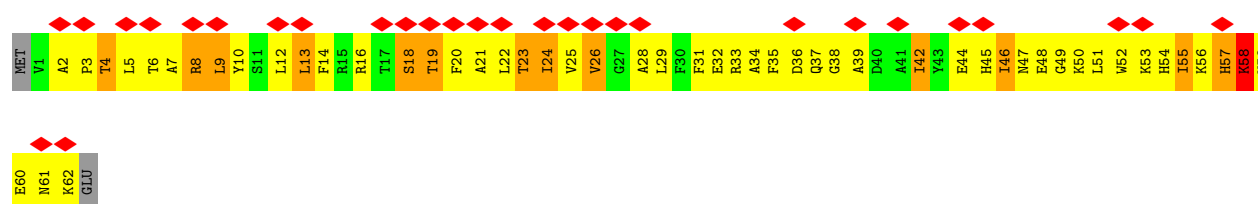
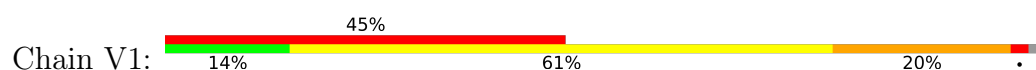
- Molecule 9: Cytochrome b-c1 complex subunit 9



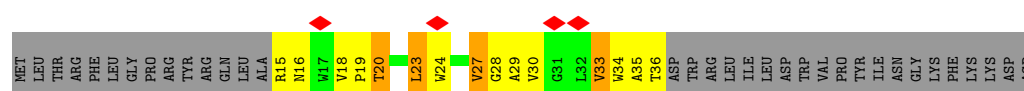
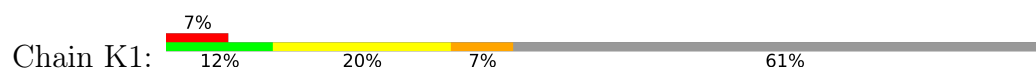
- Molecule 10: Cytochrome b-c1 complex subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 9



- Molecule 11: Cytochrome b-c1 complex subunit 10

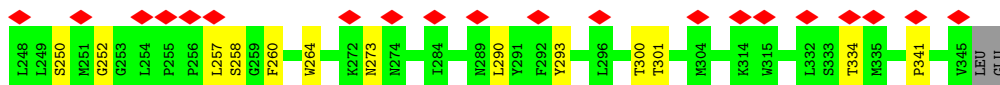
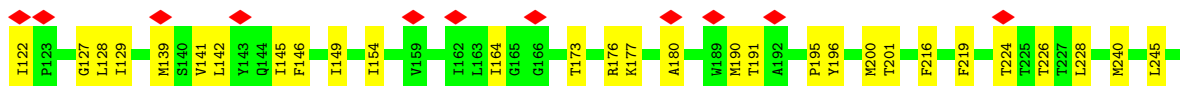
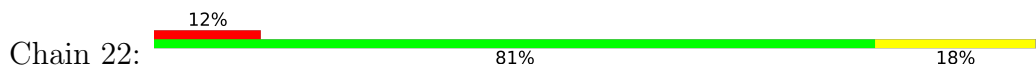


- Molecule 11: Cytochrome b-c1 complex subunit 10

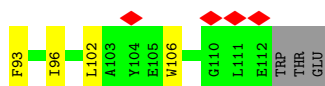
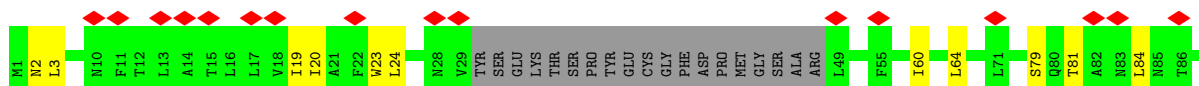




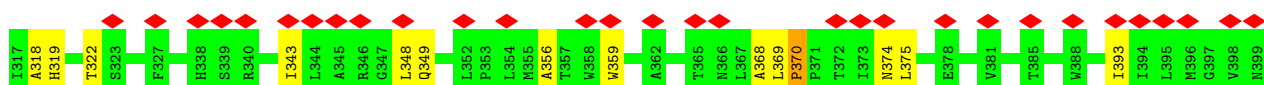
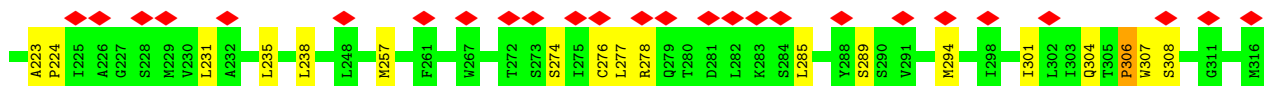
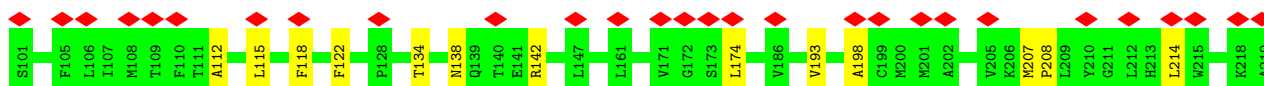
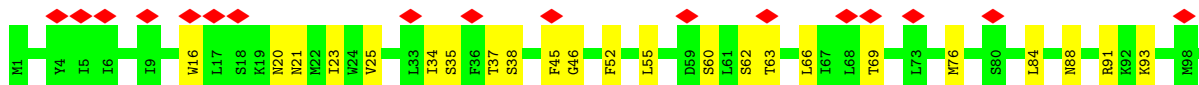
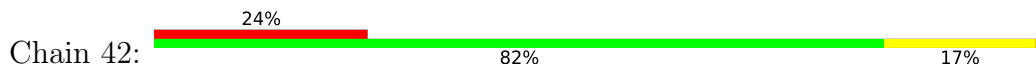
• Molecule 12: NADH-ubiquinone oxidoreductase chain 2

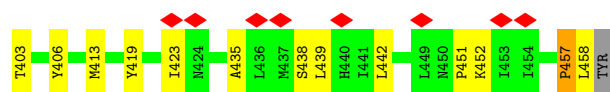


• Molecule 13: NADH-ubiquinone oxidoreductase chain 3

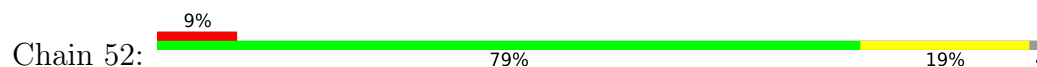


• Molecule 14: NADH-ubiquinone oxidoreductase chain 4

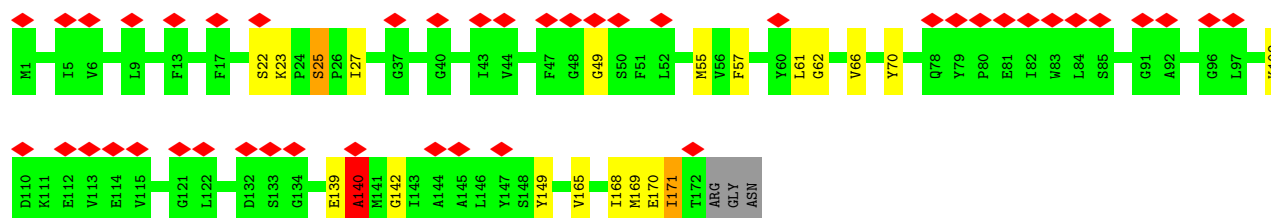
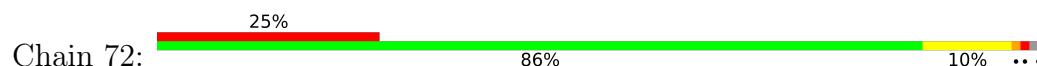




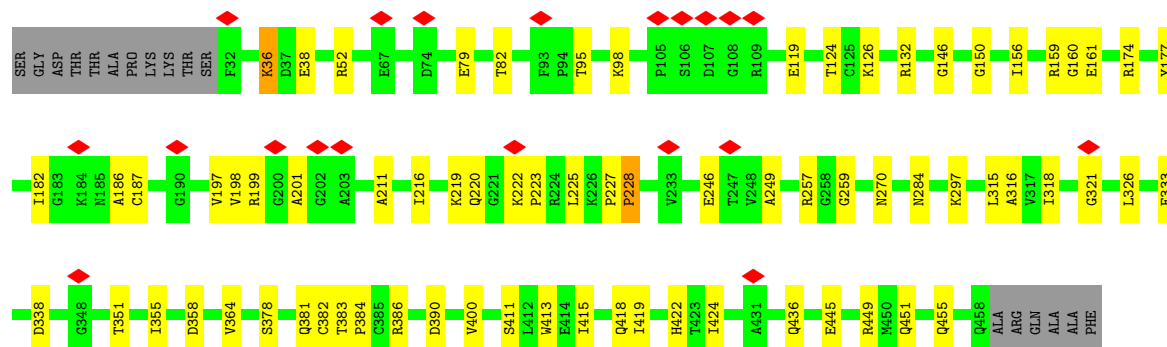
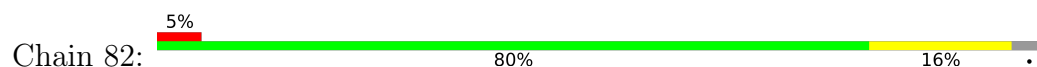
- Molecule 15: NADH-ubiquinone oxidoreductase chain 4L



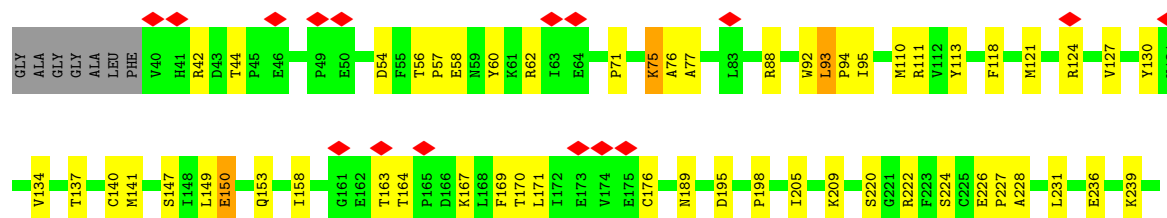
- Molecule 16: NADH-ubiquinone oxidoreductase chain 6

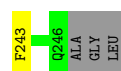


- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



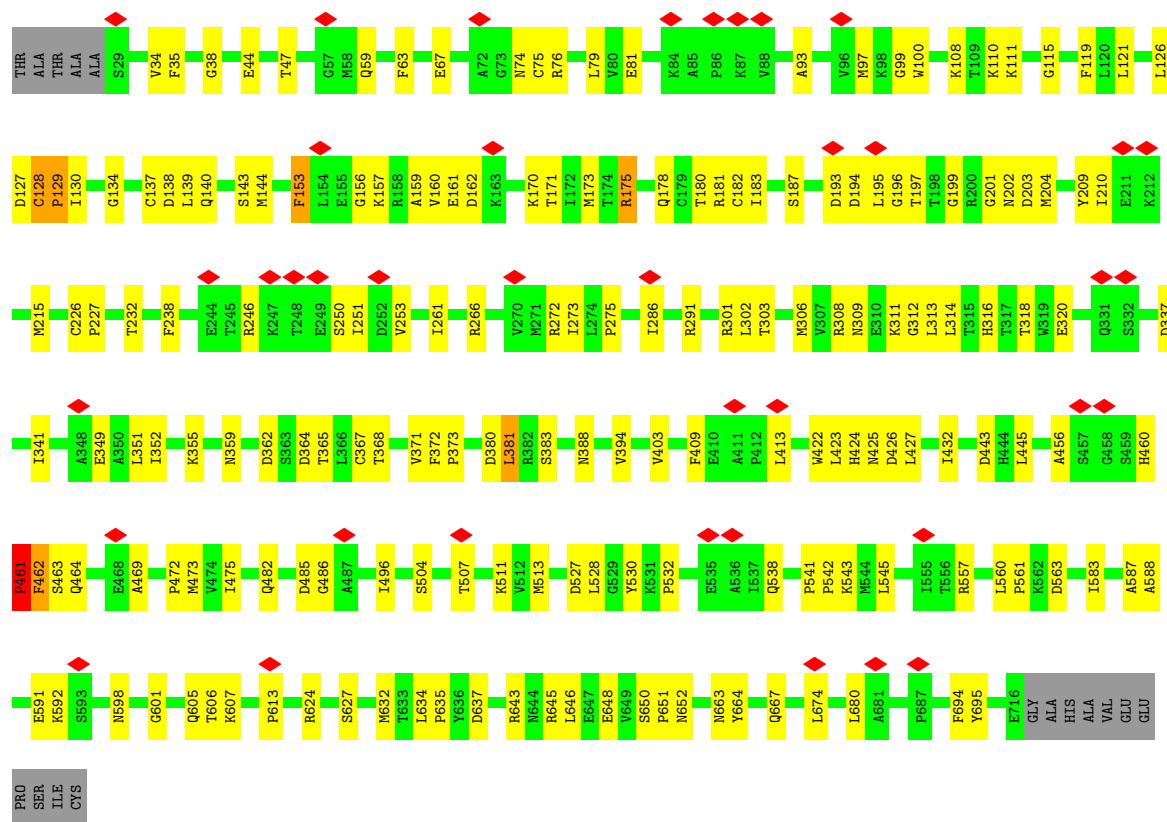
- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





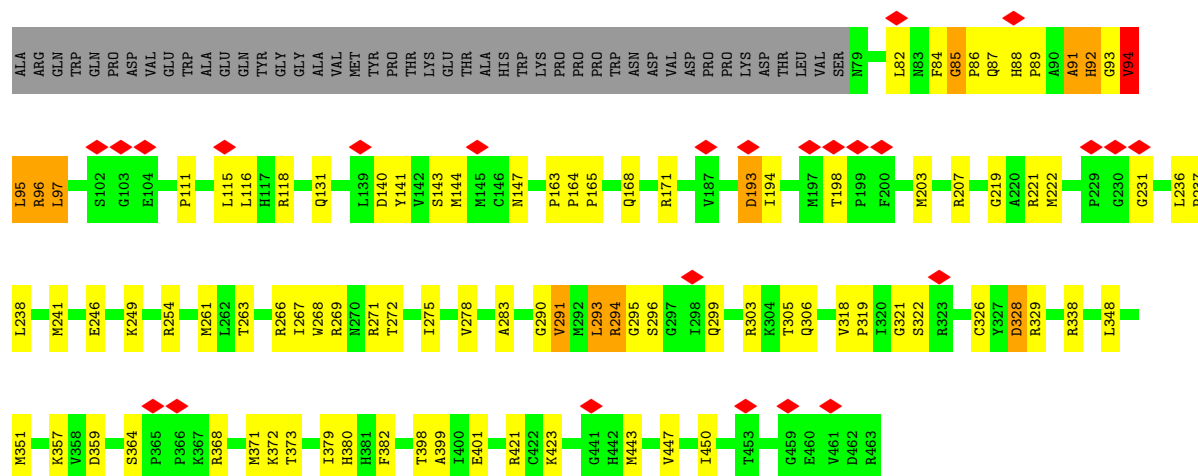
- Molecule 19: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A2: 



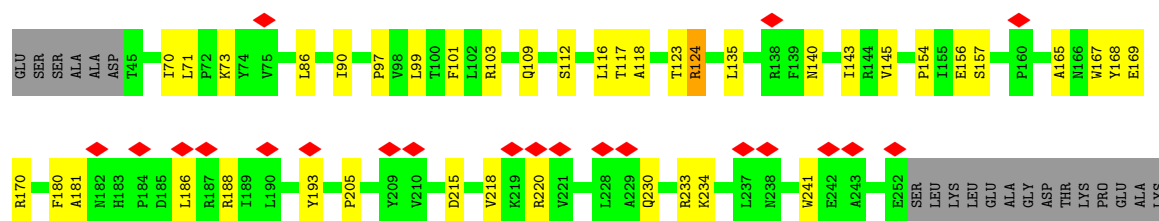
- Molecule 20: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B2: 



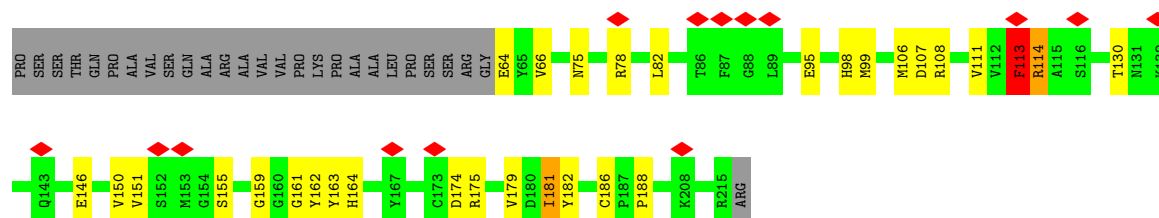
- Molecule 21: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C2: 



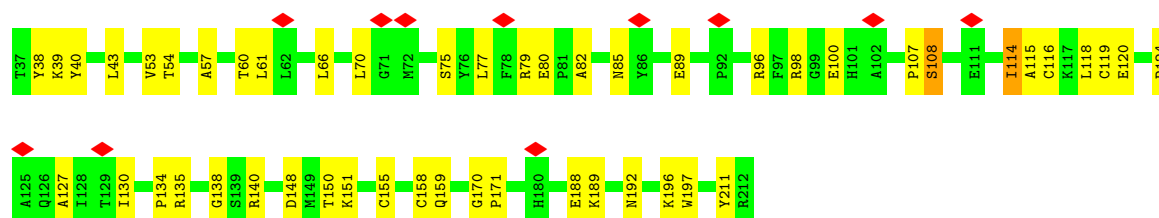
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D2: 



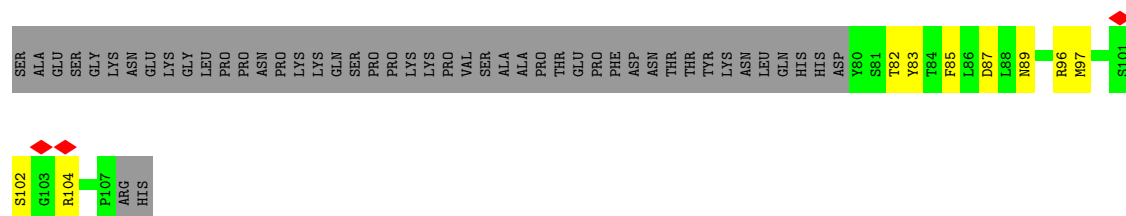
- Molecule 23: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E2: 



- Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

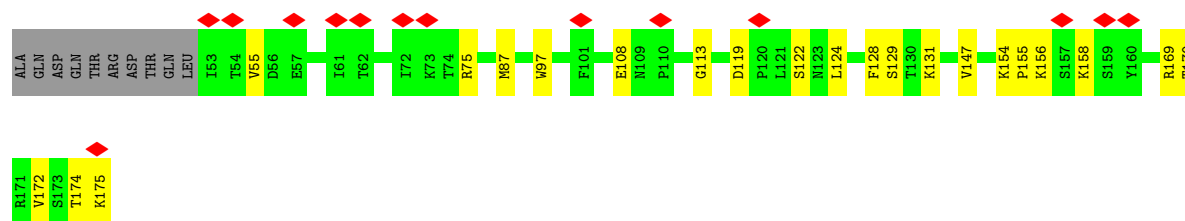
Chain F2: 



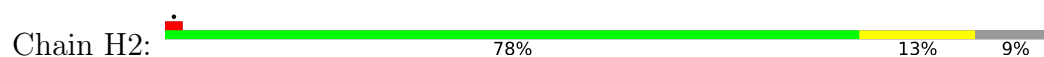
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G2: 

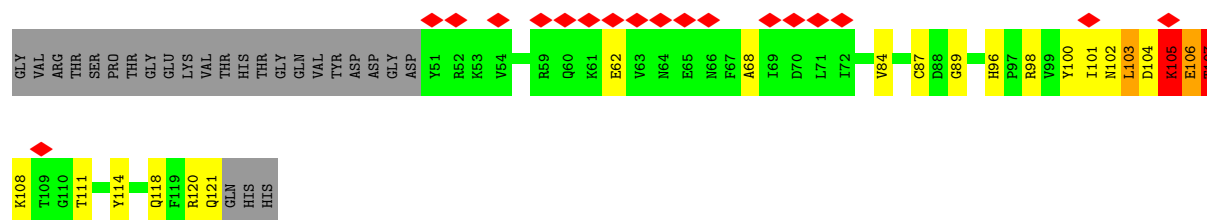




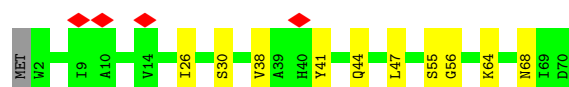
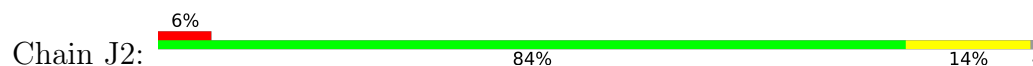
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



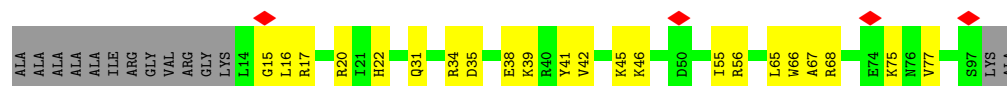
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



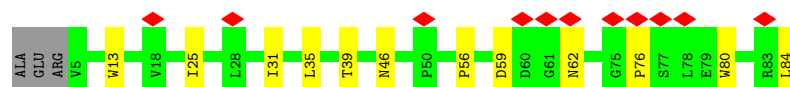
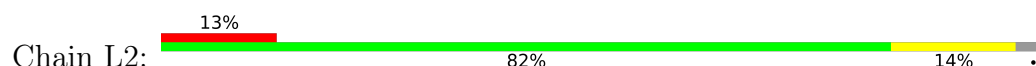
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



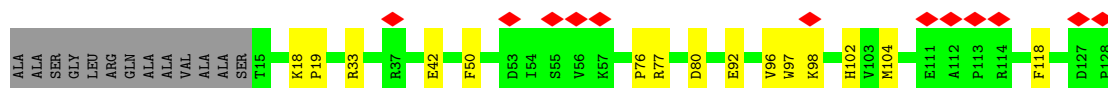
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N2:  83% 14%



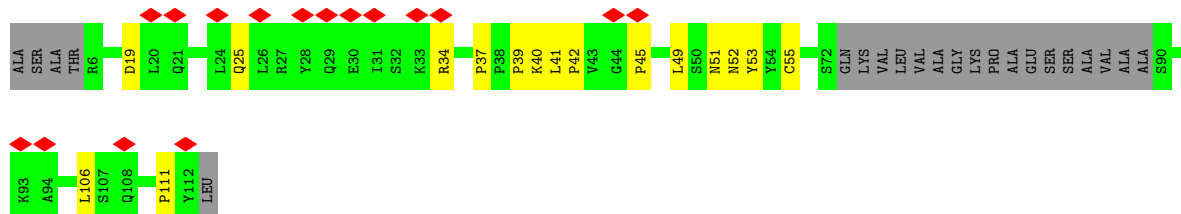
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O2:  9% 78% 12% 10%



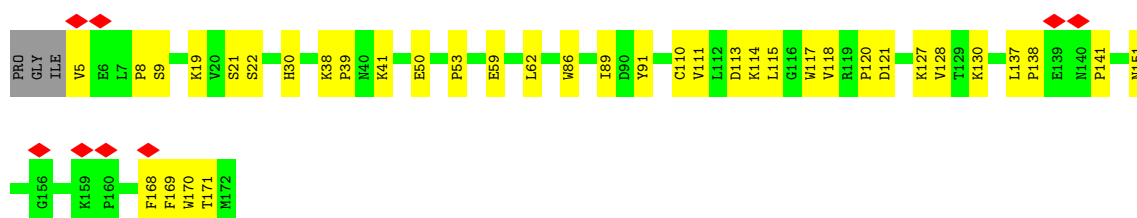
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P2:  14% 66% 14% 20%



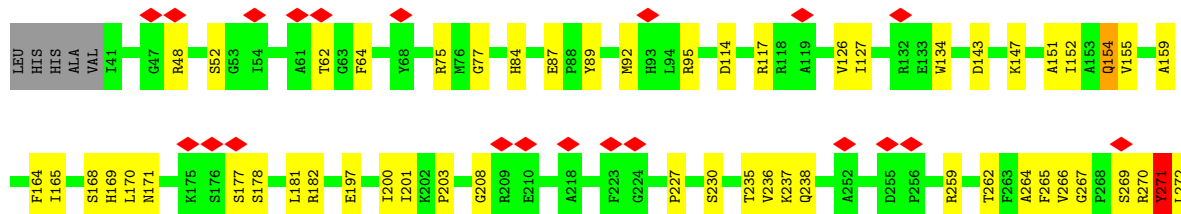
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

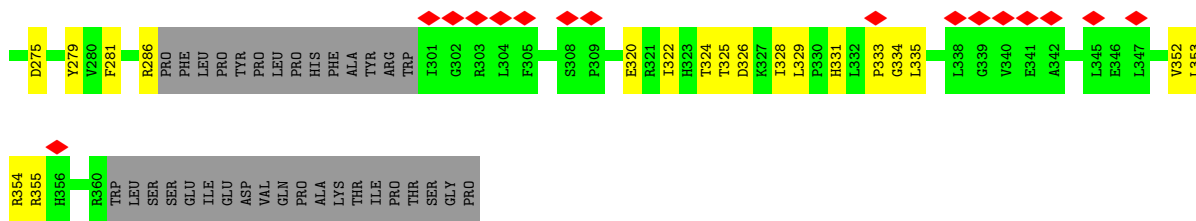
Chain Q2:  5% 77% 22%



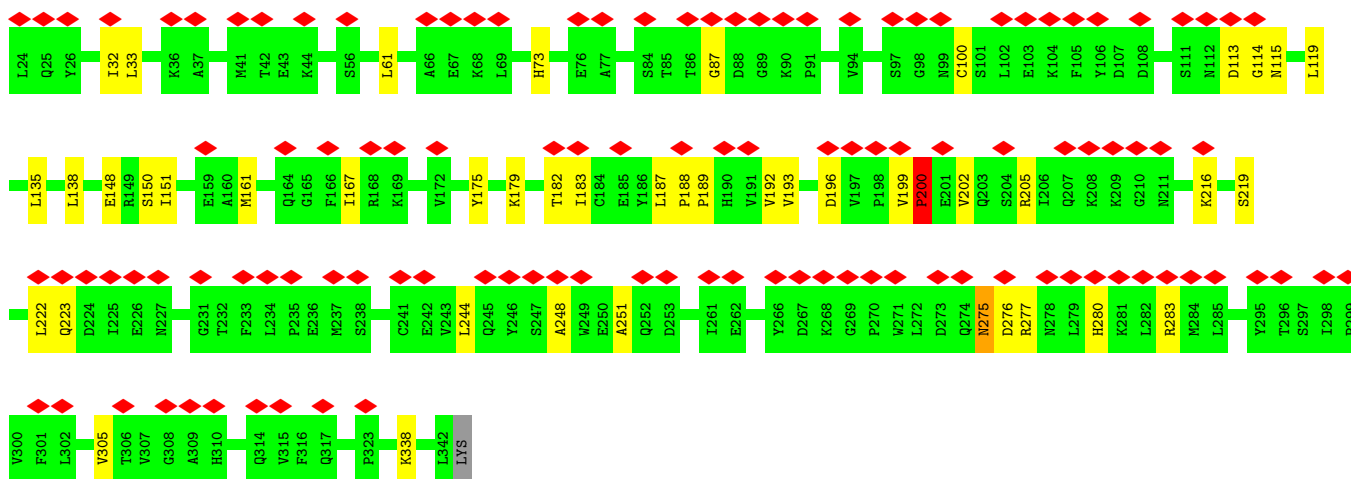
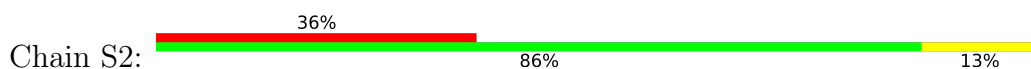
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R2:  11% 68% 21% 11%

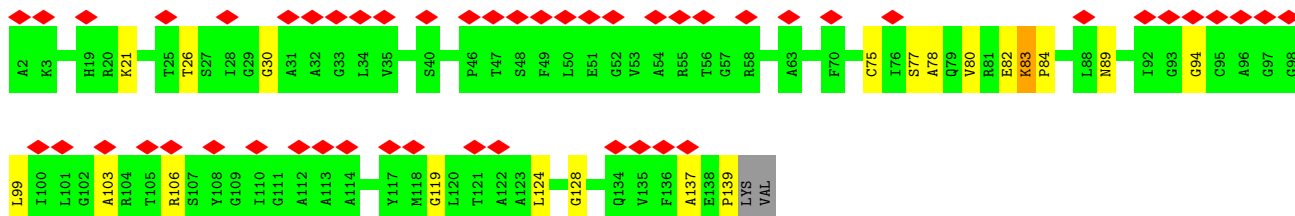
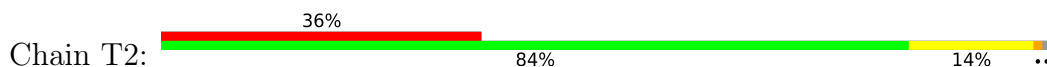




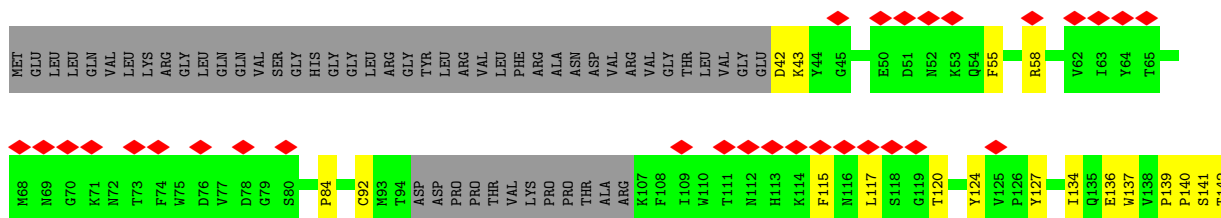
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

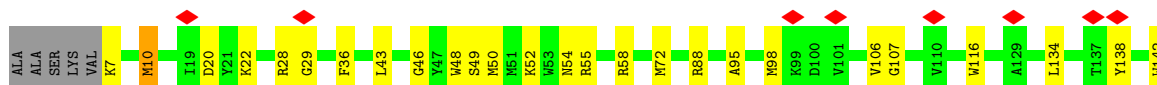
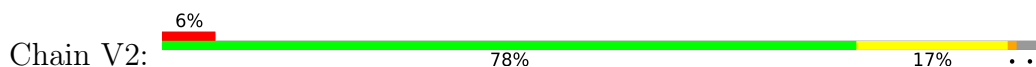


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

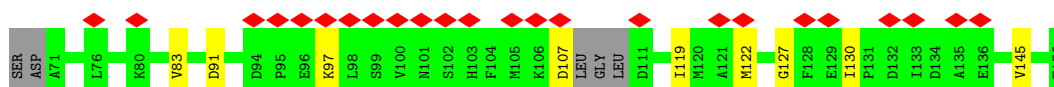
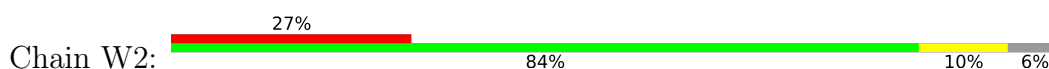




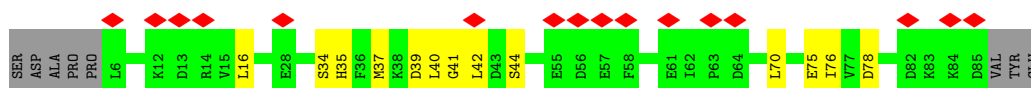
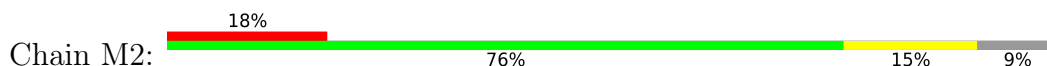
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



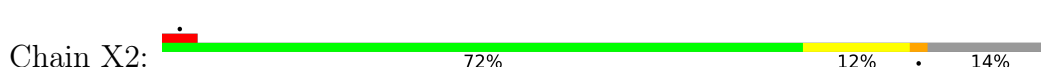
- Molecule 40: Acyl carrier protein, mitochondrial



- Molecule 40: Acyl carrier protein, mitochondrial



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



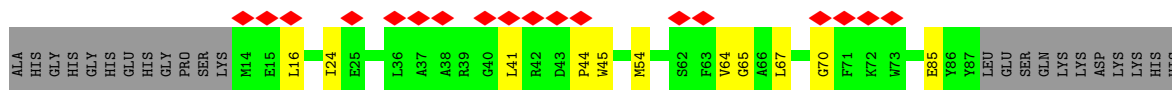
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



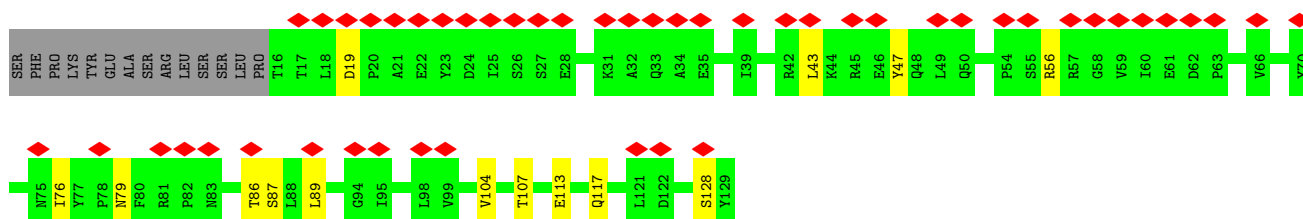
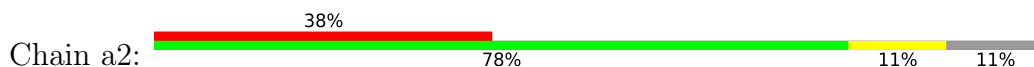
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



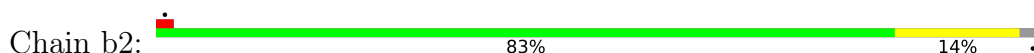




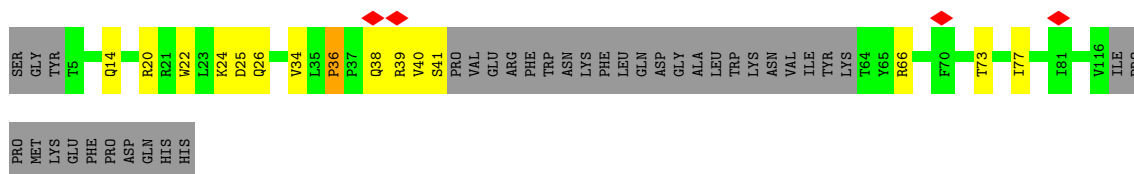
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



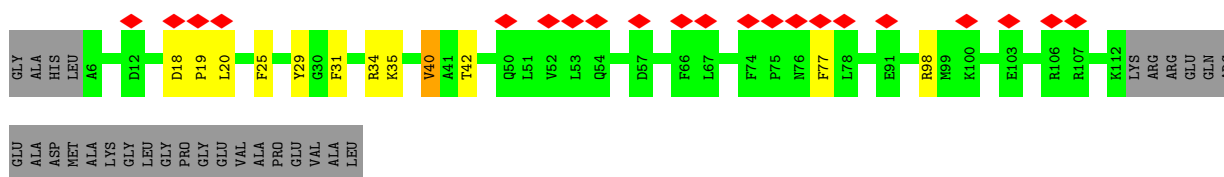
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



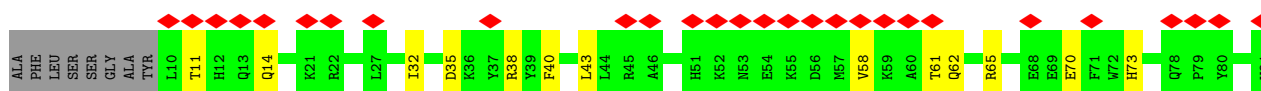
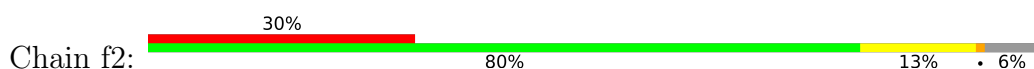
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

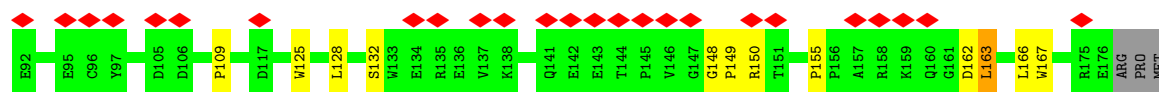


- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

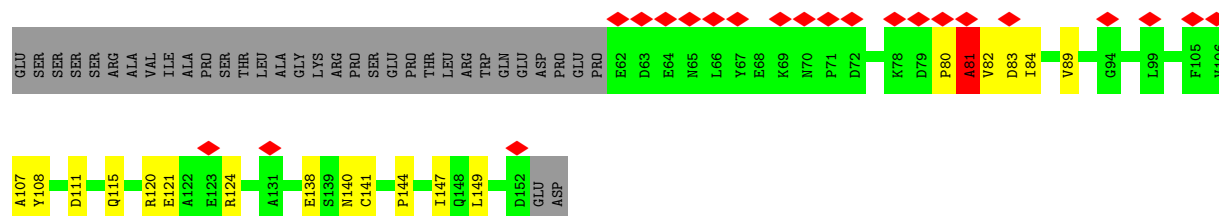


- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

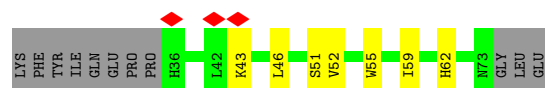




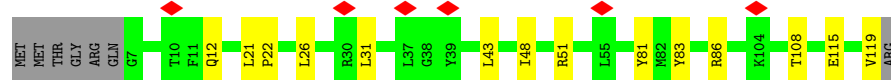
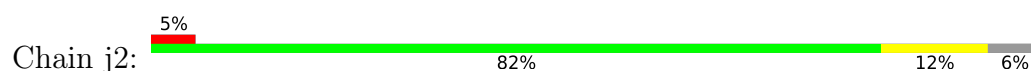
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



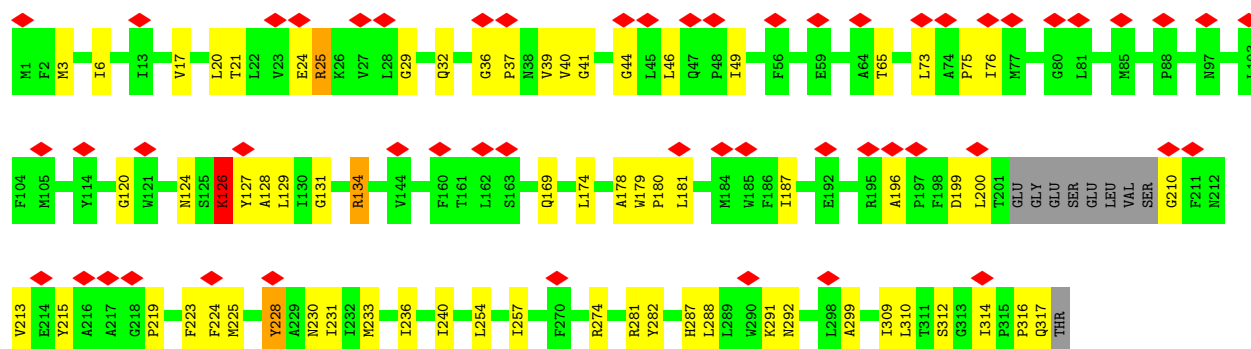
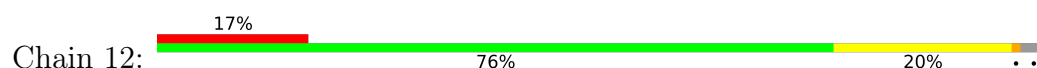
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



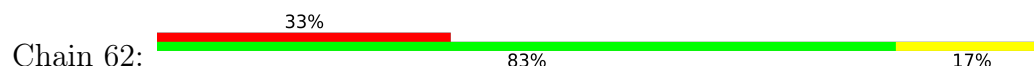
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 subunit C2

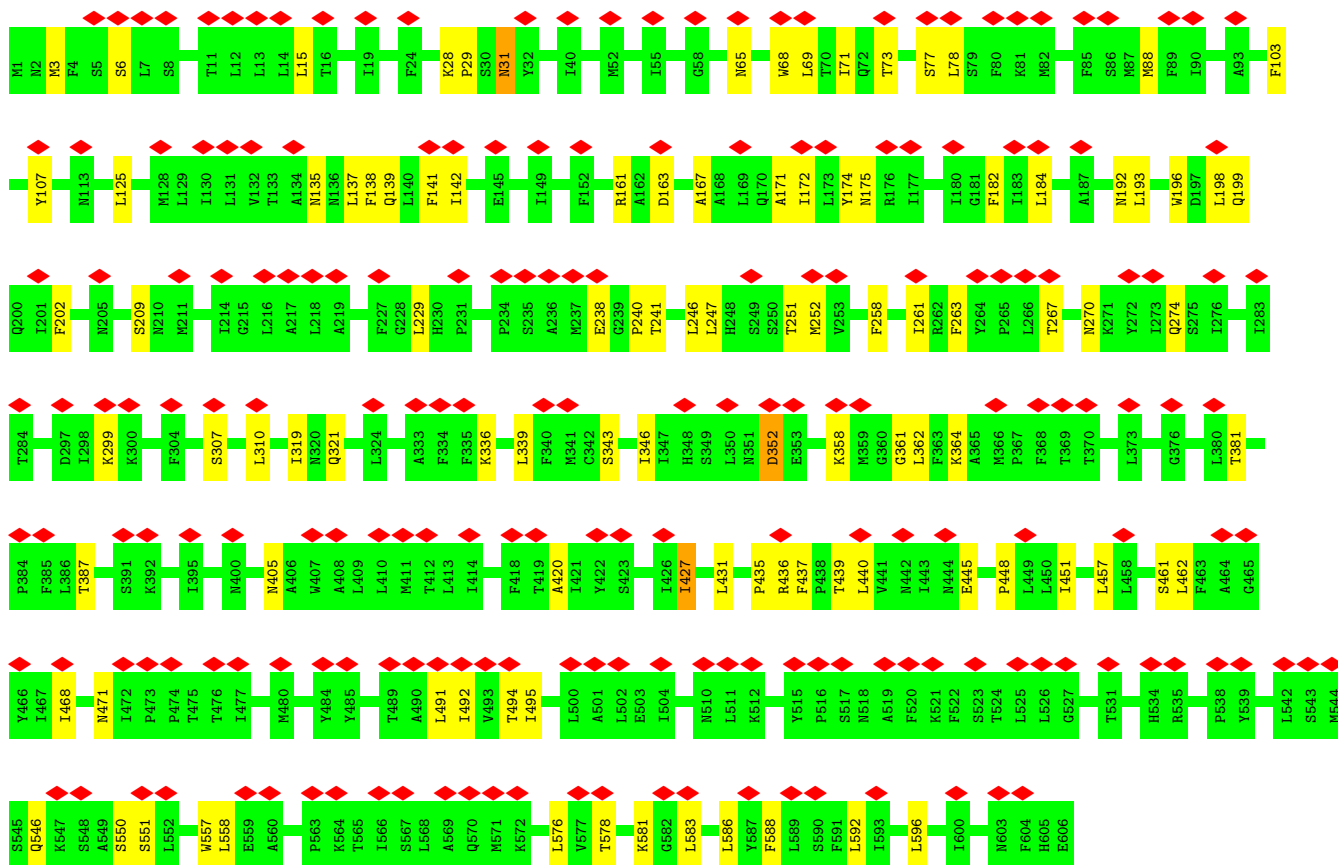


- Molecule 52: NADH-ubiquinone oxidoreductase chain 1

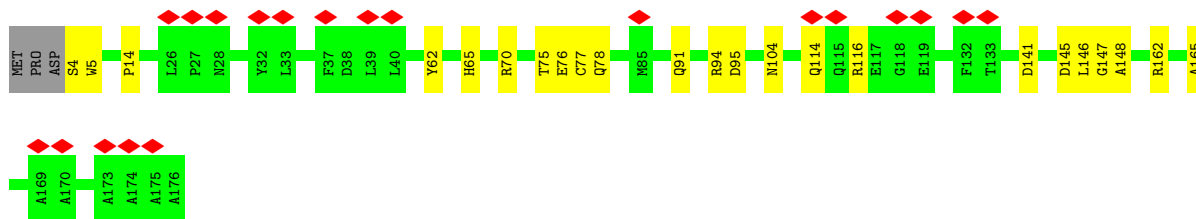
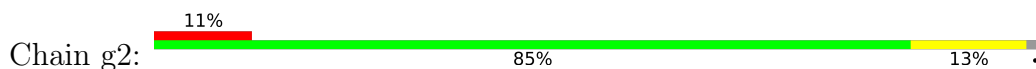


- Molecule 53: NADH-ubiquinone oxidoreductase chain 5

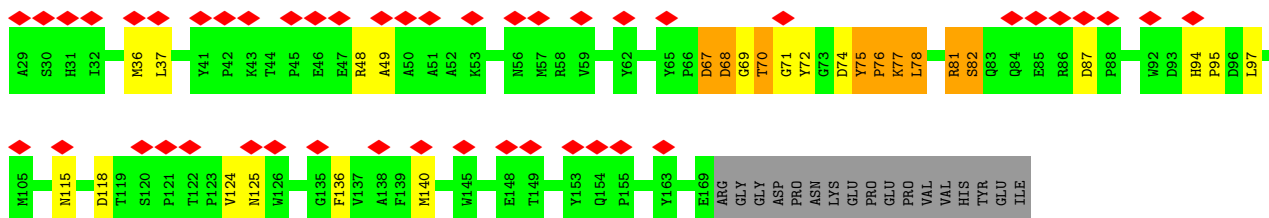
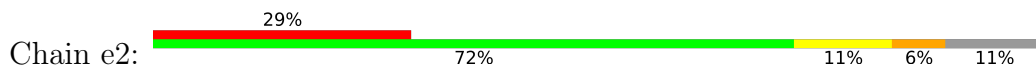




• Molecule 54: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

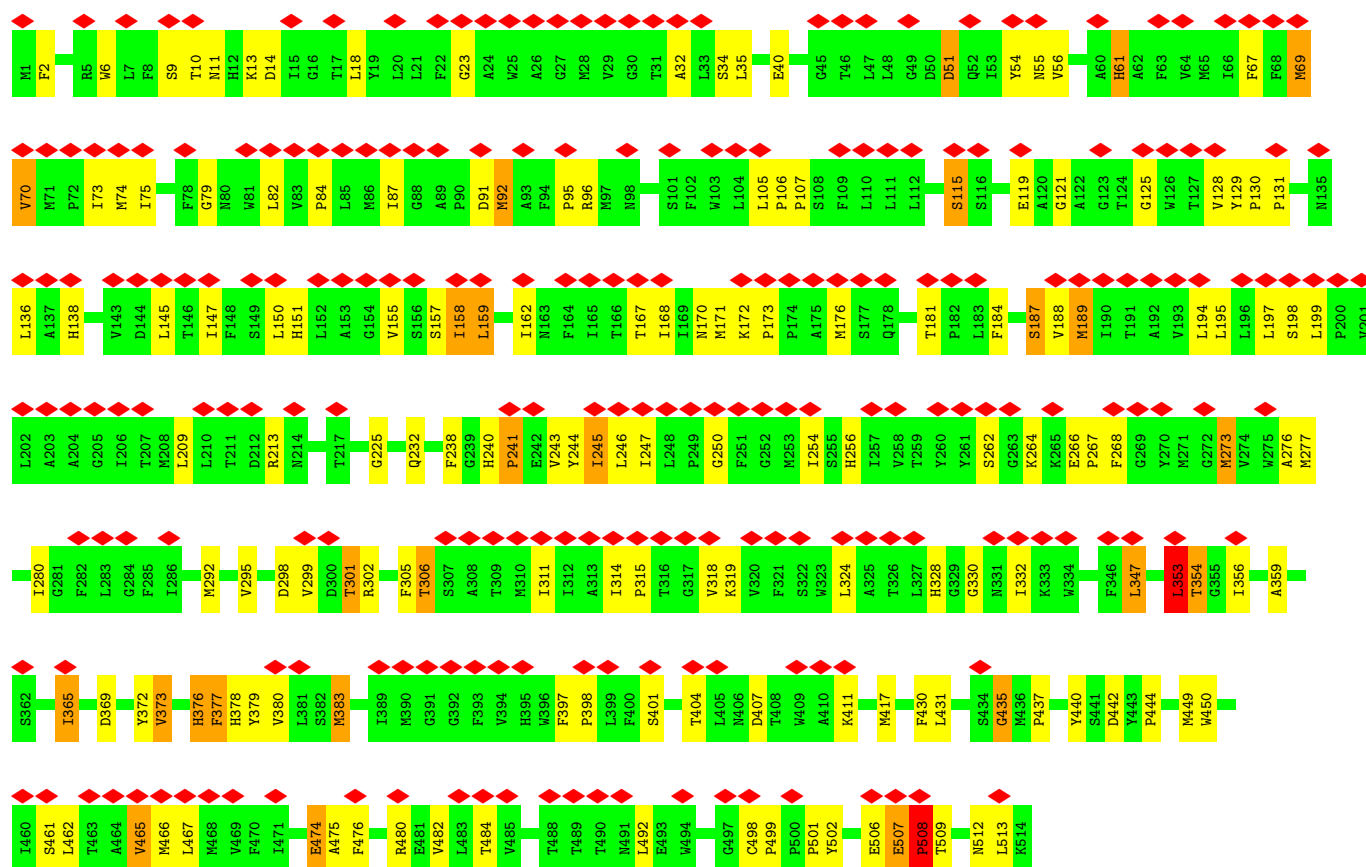


• Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



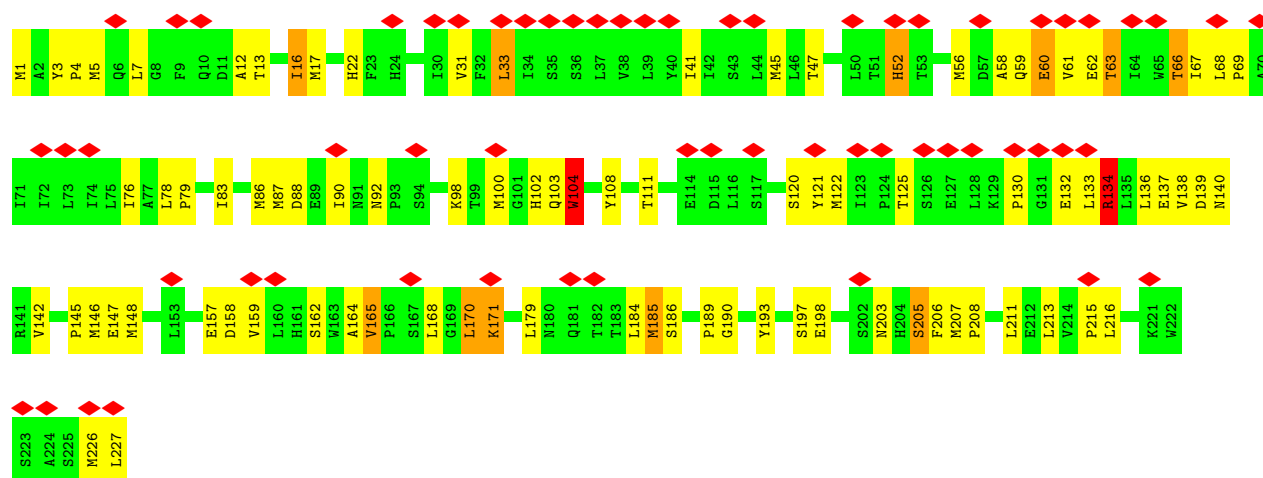
• Molecule 56: Cytochrome c oxidase subunit 1

Chain A3: 



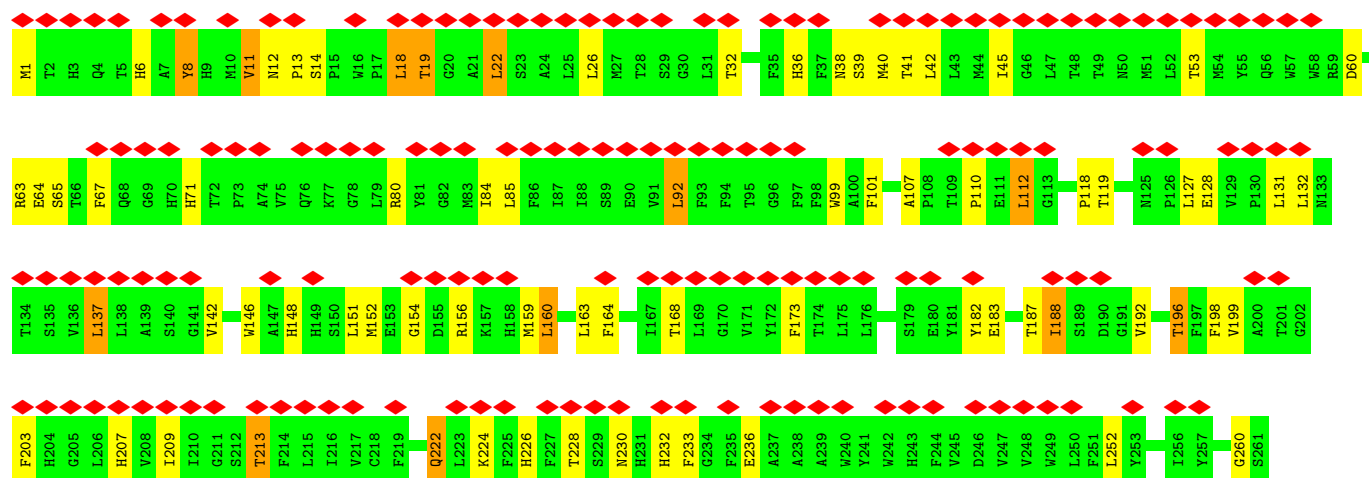
• Molecule 57: Cytochrome c oxidase subunit 2

Chain B3: 

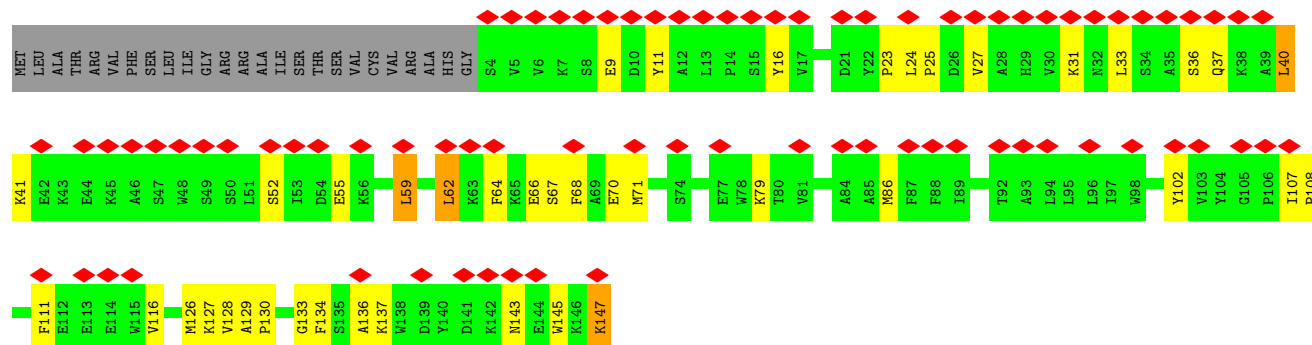


• Molecule 58: Cytochrome c oxidase subunit 3

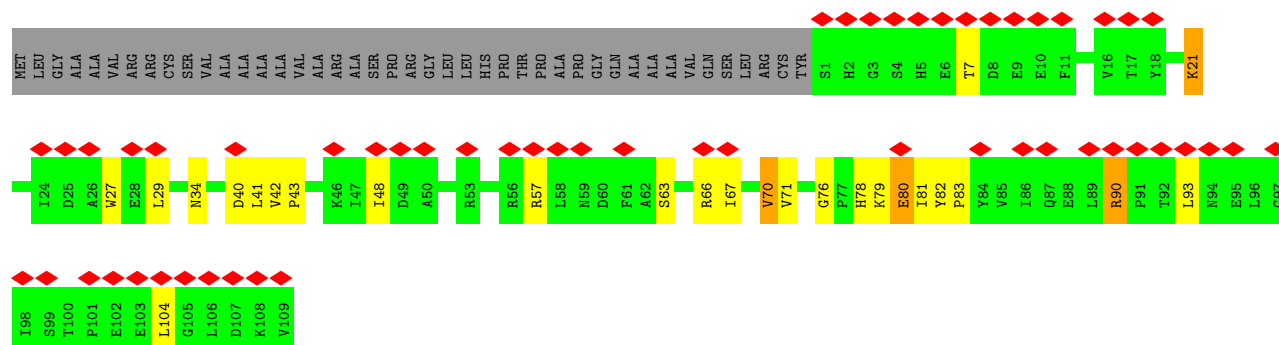
Chain C3: 



- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

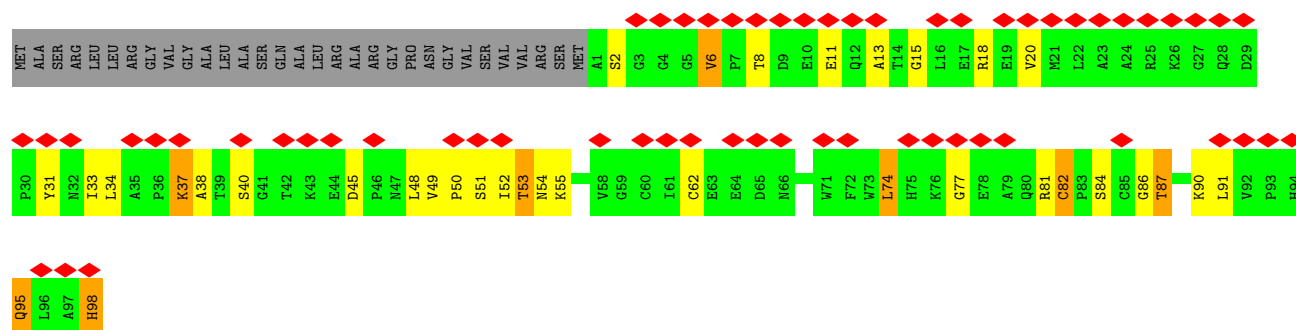


- Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

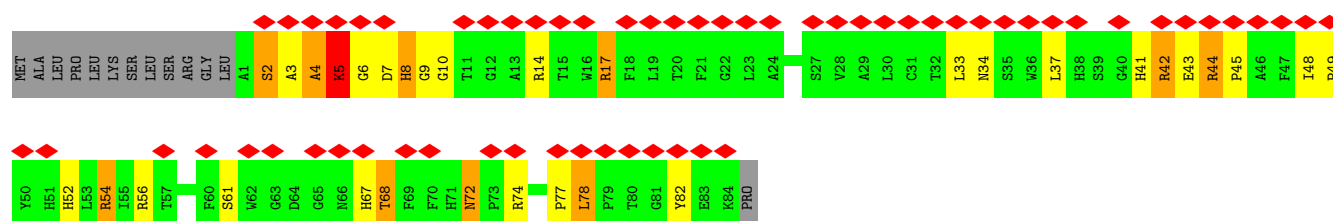


- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial

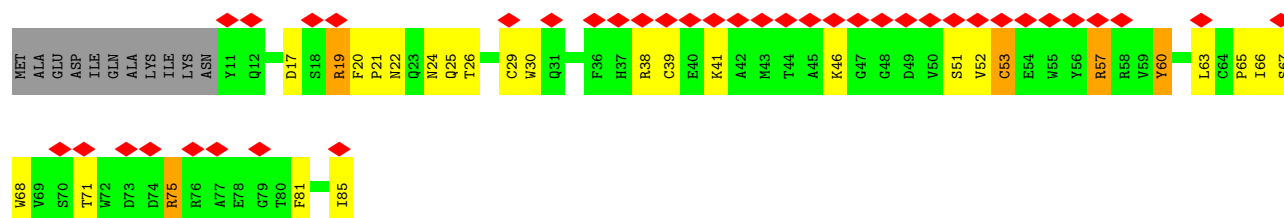




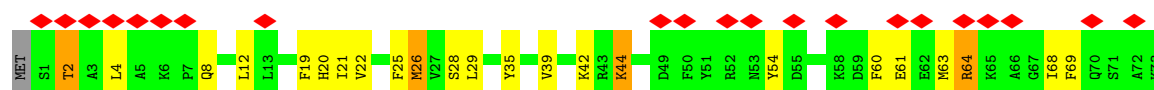
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 63: Cytochrome c oxidase subunit 6B1

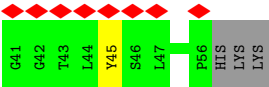


- Molecule 64: Cytochrome c oxidase subunit 6C

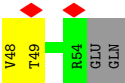


- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial





• Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 11651                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                        | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | FEI FALCON II (4k x 4k)   | Depositor |
| Maximum map value                    | 0.334                     | Depositor |
| Minimum map value                    | -0.125                    | Depositor |
| Average map value                    | 0.005                     | Depositor |
| Map value standard deviation         | 0.020                     | Depositor |
| Recommended contour level            | 0.07                      | Depositor |
| Map size ( $\text{\AA}$ )            | 391.244, 391.244, 391.244 | wwPDB     |
| Map dimensions                       | 280, 280, 280             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.3973, 1.3973, 1.3973    | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, CDL, HEM, SF4, CU, ZN, HEA, 3PE, NAP, PC1, MG, FMN

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   | A1    | 0.78         | 3/3426 (0.1%) | 2.03        | 135/4644 (2.9%) |
| 1   | M1    | 0.83         | 4/3426 (0.1%) | 2.04        | 113/4644 (2.4%) |
| 2   | B1    | 0.67         | 2/3198 (0.1%) | 1.89        | 85/4336 (2.0%)  |
| 2   | N1    | 0.65         | 0/3198        | 1.81        | 69/4336 (1.6%)  |
| 3   | C1    | 0.92         | 2/3108 (0.1%) | 2.20        | 137/4252 (3.2%) |
| 3   | O1    | 0.93         | 6/3108 (0.2%) | 2.07        | 110/4252 (2.6%) |
| 4   | D1    | 0.68         | 0/1978        | 1.88        | 55/2684 (2.0%)  |
| 4   | P1    | 0.70         | 2/1978 (0.1%) | 1.83        | 54/2684 (2.0%)  |
| 5   | E1    | 0.76         | 0/574         | 2.03        | 15/775 (1.9%)   |
| 5   | Q1    | 0.80         | 1/1551 (0.1%) | 2.16        | 63/2097 (3.0%)  |
| 6   | F1    | 0.74         | 1/935 (0.1%)  | 1.83        | 22/1253 (1.8%)  |
| 6   | R1    | 0.73         | 0/935         | 1.94        | 23/1253 (1.8%)  |
| 7   | G1    | 0.73         | 0/704         | 1.89        | 25/951 (2.6%)   |
| 7   | S1    | 0.74         | 0/704         | 1.77        | 23/951 (2.4%)   |
| 8   | H1    | 0.57         | 0/529         | 1.61        | 10/708 (1.4%)   |
| 8   | T1    | 0.50         | 0/529         | 1.51        | 4/708 (0.6%)    |
| 9   | I1    | 0.61         | 0/250         | 1.87        | 5/335 (1.5%)    |
| 9   | U1    | 0.63         | 0/250         | 1.85        | 7/335 (2.1%)    |
| 10  | J1    | 0.61         | 0/524         | 1.61        | 8/707 (1.1%)    |
| 10  | V1    | 0.63         | 0/524         | 1.71        | 7/707 (1.0%)    |
| 11  | K1    | 0.53         | 0/170         | 1.37        | 1/236 (0.4%)    |
| 11  | W1    | 0.58         | 0/170         | 1.48        | 1/236 (0.4%)    |
| 12  | 22    | 0.35         | 0/2646        | 0.77        | 8/3618 (0.2%)   |
| 13  | 32    | 0.33         | 0/736         | 0.91        | 3/1011 (0.3%)   |
| 14  | 42    | 0.31         | 0/3538        | 0.75        | 4/4845 (0.1%)   |
| 15  | 52    | 0.33         | 0/706         | 0.75        | 0/960           |
| 16  | 72    | 0.29         | 0/1213        | 0.75        | 5/1659 (0.3%)   |
| 17  | 82    | 0.28         | 0/3035        | 0.73        | 6/4130 (0.1%)   |
| 18  | 92    | 0.27         | 0/1572        | 0.69        | 0/2150          |
| 19  | A2    | 0.33         | 0/5269        | 0.71        | 10/7152 (0.1%)  |
| 20  | B2    | 0.40         | 0/3150        | 0.77        | 3/4260 (0.1%)   |
| 21  | C2    | 0.33         | 0/1756        | 0.69        | 2/2394 (0.1%)   |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 22  | D2    | 0.37         | 0/1231        | 0.67        | 0/1669         |
| 23  | E2    | 0.37         | 0/1418        | 0.76        | 3/1922 (0.2%)  |
| 24  | F2    | 0.36         | 0/188         | 1.31        | 5/259 (1.9%)   |
| 25  | G2    | 0.33         | 0/1004        | 0.78        | 4/1359 (0.3%)  |
| 26  | H2    | 0.30         | 0/800         | 0.69        | 0/1076         |
| 27  | I2    | 0.27         | 0/540         | 0.84        | 2/725 (0.3%)   |
| 28  | J2    | 0.25         | 0/545         | 0.54        | 0/740          |
| 29  | K2    | 0.27         | 0/663         | 0.67        | 0/896          |
| 30  | L2    | 0.30         | 0/623         | 0.80        | 4/862 (0.5%)   |
| 31  | N2    | 0.27         | 0/882         | 0.71        | 0/1203         |
| 32  | O2    | 0.26         | 0/948         | 0.66        | 4/1279 (0.3%)  |
| 33  | P2    | 0.29         | 0/719         | 0.79        | 1/981 (0.1%)   |
| 34  | Q2    | 0.28         | 0/1381        | 0.78        | 2/1869 (0.1%)  |
| 35  | R2    | 0.28         | 0/2392        | 0.78        | 5/3248 (0.2%)  |
| 36  | S2    | 0.28         | 0/2348        | 0.78        | 6/3198 (0.2%)  |
| 37  | T2    | 0.26         | 0/959         | 0.70        | 1/1305 (0.1%)  |
| 38  | U2    | 0.29         | 0/765         | 0.82        | 3/1050 (0.3%)  |
| 39  | V2    | 0.29         | 0/1121        | 0.66        | 0/1515         |
| 40  | M2    | 0.24         | 0/651         | 0.79        | 0/876          |
| 40  | W2    | 0.24         | 0/603         | 0.73        | 0/817          |
| 41  | X2    | 0.27         | 0/383         | 0.86        | 2/523 (0.4%)   |
| 42  | Y2    | 0.27         | 0/428         | 0.64        | 0/592          |
| 43  | Z2    | 0.30         | 0/506         | 0.90        | 4/688 (0.6%)   |
| 44  | a2    | 0.25         | 0/878         | 0.72        | 4/1195 (0.3%)  |
| 45  | b2    | 0.29         | 0/1058        | 0.71        | 0/1434         |
| 46  | c2    | 0.32         | 0/632         | 0.94        | 5/871 (0.6%)   |
| 47  | d2    | 0.33         | 0/724         | 0.69        | 2/989 (0.2%)   |
| 48  | f2    | 0.24         | 0/1191        | 0.71        | 2/1639 (0.1%)  |
| 49  | h2    | 0.29         | 0/743         | 0.78        | 0/1013         |
| 50  | i2    | 0.20         | 0/286         | 0.44        | 0/392          |
| 51  | j2    | 0.28         | 0/922         | 0.78        | 5/1254 (0.4%)  |
| 52  | l2    | 0.35         | 0/2513        | 0.78        | 1/3432 (0.0%)  |
| 53  | 62    | 0.25         | 0/4892        | 0.65        | 2/6660 (0.0%)  |
| 54  | g2    | 0.25         | 0/1380        | 0.65        | 0/1872         |
| 55  | e2    | 0.40         | 0/888         | 1.05        | 6/1234 (0.5%)  |
| 56  | A3    | 0.86         | 7/4164 (0.2%) | 1.16        | 36/5688 (0.6%) |
| 57  | B3    | 0.77         | 0/1868        | 1.12        | 10/2544 (0.4%) |
| 58  | C3    | 0.74         | 0/2211        | 1.01        | 7/3023 (0.2%)  |
| 59  | D3    | 0.67         | 0/1229        | 0.96        | 3/1658 (0.2%)  |
| 60  | E3    | 0.64         | 0/898         | 1.03        | 6/1218 (0.5%)  |
| 61  | F3    | 0.72         | 0/765         | 1.13        | 4/1038 (0.4%)  |
| 62  | G3    | 0.69         | 0/698         | 1.09        | 6/950 (0.6%)   |
| 63  | H3    | 0.68         | 0/648         | 1.18        | 5/877 (0.6%)   |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 64  | I3    | 0.71         | 0/611            | 0.94        | 2/810 (0.2%)       |
| 65  | J3    | 0.70         | 0/451            | 1.04        | 3/610 (0.5%)       |
| 66  | K3    | 0.75         | 0/398            | 1.01        | 0/546              |
| 67  | L3    | 0.77         | 0/399            | 0.98        | 2/534 (0.4%)       |
| 68  | M3    | 0.69         | 0/345            | 0.98        | 1/470 (0.2%)       |
| All | All   | 0.55         | 28/107280 (0.0%) | 1.27        | 1171/145866 (0.8%) |

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   | A1    | 0                   | 13                  |
| 1   | M1    | 0                   | 3                   |
| 2   | B1    | 0                   | 9                   |
| 2   | N1    | 0                   | 6                   |
| 3   | C1    | 0                   | 14                  |
| 3   | O1    | 0                   | 6                   |
| 4   | D1    | 0                   | 5                   |
| 4   | P1    | 0                   | 4                   |
| 5   | E1    | 0                   | 1                   |
| 5   | Q1    | 0                   | 9                   |
| 6   | F1    | 0                   | 2                   |
| 7   | G1    | 0                   | 2                   |
| 7   | S1    | 0                   | 3                   |
| 8   | T1    | 0                   | 1                   |
| 9   | I1    | 0                   | 1                   |
| 9   | U1    | 0                   | 1                   |
| 10  | J1    | 0                   | 1                   |
| 11  | W1    | 0                   | 1                   |
| 12  | 22    | 0                   | 2                   |
| 14  | 42    | 0                   | 3                   |
| 15  | 52    | 0                   | 1                   |
| 16  | 72    | 0                   | 3                   |
| 17  | 82    | 0                   | 1                   |
| 18  | 92    | 0                   | 3                   |
| 19  | A2    | 0                   | 6                   |
| 20  | B2    | 0                   | 3                   |
| 22  | D2    | 0                   | 4                   |
| 23  | E2    | 0                   | 2                   |
| 33  | P2    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 34  | Q2    | 0                   | 2                   |
| 35  | R2    | 0                   | 2                   |
| 36  | S2    | 0                   | 1                   |
| 37  | T2    | 0                   | 1                   |
| 39  | V2    | 0                   | 3                   |
| 40  | M2    | 0                   | 1                   |
| 42  | Y2    | 0                   | 1                   |
| 45  | b2    | 0                   | 1                   |
| 48  | f2    | 0                   | 1                   |
| 49  | h2    | 0                   | 2                   |
| 52  | 12    | 0                   | 1                   |
| 53  | 62    | 0                   | 2                   |
| 55  | e2    | 0                   | 4                   |
| All | All   | 0                   | 133                 |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M1    | 253 | VAL  | C-O     | 11.17 | 1.36        | 1.24     |
| 3   | O1    | 37  | LEU  | C-N     | -8.10 | 1.24        | 1.33     |
| 56  | A3    | 61  | HIS  | CG-CD2  | 7.61  | 1.44        | 1.35     |
| 56  | A3    | 378 | HIS  | ND1-CE1 | 7.16  | 1.39        | 1.32     |
| 3   | O1    | 221 | HIS  | CD2-NE2 | -7.09 | 1.30        | 1.37     |
| 56  | A3    | 378 | HIS  | CE1-NE2 | -6.56 | 1.25        | 1.32     |
| 4   | P1    | 202 | LYS  | C-O     | 6.45  | 1.31        | 1.24     |
| 3   | O1    | 19  | ILE  | CA-C    | -6.39 | 1.44        | 1.52     |
| 3   | O1    | 44  | GLN  | C-N     | -6.34 | 1.26        | 1.33     |
| 56  | A3    | 69  | MET  | SD-CE   | -6.27 | 1.63        | 1.79     |
| 1   | M1    | 169 | GLY  | N-CA    | -6.18 | 1.36        | 1.44     |
| 3   | O1    | 185 | LEU  | CA-CB   | -6.11 | 1.45        | 1.53     |
| 1   | A1    | 153 | LEU  | N-CA    | -6.10 | 1.39        | 1.46     |
| 3   | O1    | 328 | LEU  | C-N     | 5.90  | 1.41        | 1.33     |
| 1   | M1    | 340 | GLY  | C-O     | -5.81 | 1.16        | 1.23     |
| 2   | B1    | 148 | LYS  | C-N     | -5.79 | 1.26        | 1.33     |
| 3   | C1    | 97  | HIS  | C-O     | -5.56 | 1.17        | 1.24     |
| 1   | A1    | 373 | THR  | C-O     | 5.56  | 1.29        | 1.24     |
| 56  | A3    | 61  | HIS  | ND1-CE1 | 5.55  | 1.38        | 1.32     |
| 5   | Q1    | 55  | VAL  | C-O     | -5.54 | 1.17        | 1.24     |
| 3   | C1    | 126 | THR  | N-CA    | -5.51 | 1.39        | 1.46     |
| 56  | A3    | 376 | HIS  | ND1-CE1 | 5.49  | 1.38        | 1.32     |
| 6   | F1    | 68  | LEU  | C-O     | -5.49 | 1.17        | 1.24     |
| 56  | A3    | 378 | HIS  | CG-CD2  | 5.46  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | M1    | 333 | ASP  | C-O   | -5.31 | 1.18        | 1.24     |
| 4   | P1    | 228 | SER  | C-N   | -5.22 | 1.27        | 1.33     |
| 1   | A1    | 104 | LYS  | CD-CE | 5.07  | 1.67        | 1.52     |
| 2   | B1    | 173 | ALA  | CA-CB | -5.04 | 1.44        | 1.53     |

All (1171) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | M1    | 253 | VAL  | O-C-N       | -23.38 | 98.86       | 123.18   |
| 1   | M1    | 253 | VAL  | CA-C-O      | 16.98  | 137.42      | 120.27   |
| 3   | C1    | 196 | HIS  | CA-CB-CG    | 16.18  | 129.98      | 113.80   |
| 3   | O1    | 196 | HIS  | CA-CB-CG    | 15.64  | 129.44      | 113.80   |
| 3   | O1    | 44  | GLN  | CA-C-N      | 15.24  | 139.75      | 120.70   |
| 3   | O1    | 44  | GLN  | C-N-CA      | 15.24  | 139.75      | 120.70   |
| 1   | M1    | 168 | GLU  | CA-C-N      | 14.27  | 144.28      | 121.87   |
| 1   | M1    | 168 | GLU  | C-N-CA      | 14.27  | 144.28      | 121.87   |
| 3   | C1    | 204 | GLY  | CA-C-N      | 14.20  | 142.04      | 121.02   |
| 3   | C1    | 204 | GLY  | C-N-CA      | 14.20  | 142.04      | 121.02   |
| 1   | M1    | 435 | ASN  | OD1-CG-ND2  | 13.87  | 136.47      | 122.60   |
| 1   | A1    | 168 | GLU  | CA-C-O      | 13.48  | 135.33      | 120.10   |
| 6   | R1    | 65  | ALA  | CA-C-O      | 12.87  | 134.16      | 120.90   |
| 55  | e2    | 77  | LYS  | N-CA-C      | -12.71 | 97.42       | 111.28   |
| 1   | A1    | 419 | CYS  | CA-CB-SG    | 12.53  | 143.22      | 114.40   |
| 6   | R1    | 77  | LYS  | CG-CD-CE    | 11.36  | 137.43      | 111.30   |
| 1   | A1    | 251 | ALA  | CA-C-O      | 11.32  | 132.59      | 120.36   |
| 4   | P1    | 235 | LEU  | CA-C-O      | 11.29  | 133.87      | 121.11   |
| 1   | M1    | 307 | PHE  | CA-C-O      | 11.25  | 135.40      | 120.21   |
| 3   | C1    | 267 | HIS  | CA-CB-CG    | -11.03 | 102.77      | 113.80   |
| 2   | B1    | 178 | CYS  | O-C-N       | 10.81  | 131.76      | 121.27   |
| 2   | B1    | 177 | TYR  | O-C-N       | 10.55  | 135.75      | 123.29   |
| 8   | T1    | 74  | PHE  | CA-CB-CG    | -10.44 | 103.36      | 113.80   |
| 56  | A3    | 376 | HIS  | ND1-CE1-NE2 | 10.39  | 118.79      | 108.40   |
| 3   | O1    | 47  | THR  | O-C-N       | -10.29 | 111.47      | 122.07   |
| 2   | B1    | 70  | ARG  | NE-CZ-NH2   | 10.24  | 128.42      | 119.20   |
| 3   | O1    | 267 | HIS  | CA-CB-CG    | -10.21 | 103.59      | 113.80   |
| 1   | M1    | 437 | ILE  | N-CA-C      | -10.19 | 100.78      | 111.58   |
| 1   | M1    | 334 | MET  | O-C-N       | -10.17 | 110.56      | 122.15   |
| 1   | A1    | 294 | LEU  | CA-C-N      | 10.14  | 134.69      | 120.29   |
| 1   | A1    | 294 | LEU  | C-N-CA      | 10.14  | 134.69      | 120.29   |
| 5   | E1    | 58  | PHE  | CA-CB-CG    | 10.06  | 123.86      | 113.80   |
| 7   | G1    | 13  | VAL  | CA-C-O      | 9.95   | 130.84      | 120.39   |
| 8   | H1    | 74  | PHE  | CA-CB-CG    | -9.92  | 103.88      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 9   | I1    | 75  | SER  | N-CA-C     | 9.90  | 121.00      | 107.73   |
| 3   | C1    | 196 | HIS  | CA-C-O     | -9.87 | 110.64      | 121.00   |
| 4   | P1    | 228 | SER  | CA-C-N     | 9.86  | 133.32      | 120.60   |
| 4   | P1    | 228 | SER  | C-N-CA     | 9.86  | 133.32      | 120.60   |
| 55  | e2    | 118 | ASP  | N-CA-C     | 9.61  | 122.42      | 108.86   |
| 3   | O1    | 19  | ILE  | O-C-N      | -9.60 | 110.57      | 122.57   |
| 1   | M1    | 46  | ARG  | NE-CZ-NH2  | -9.52 | 110.64      | 119.20   |
| 4   | D1    | 14  | HIS  | CA-CB-CG   | 9.49  | 123.30      | 113.80   |
| 2   | B1    | 245 | ARG  | NE-CZ-NH2  | 9.49  | 127.74      | 119.20   |
| 3   | C1    | 185 | LEU  | O-C-N      | -9.47 | 112.90      | 120.38   |
| 10  | V1    | 26  | VAL  | CA-CB-CG1  | 9.46  | 126.49      | 110.40   |
| 10  | V1    | 39  | ALA  | O-C-N      | 9.45  | 132.13      | 122.12   |
| 20  | B2    | 193 | ASP  | N-CA-C     | -9.36 | 101.06      | 111.07   |
| 1   | A1    | 373 | THR  | CA-C-O     | 9.24  | 127.12      | 118.44   |
| 3   | C1    | 41  | LEU  | N-CA-CB    | 9.21  | 123.79      | 110.16   |
| 1   | M1    | 259 | GLY  | CA-C-N     | 9.18  | 129.74      | 119.92   |
| 1   | M1    | 259 | GLY  | C-N-CA     | 9.18  | 129.74      | 119.92   |
| 2   | N1    | 56  | ARG  | CD-NE-CZ   | 9.17  | 137.24      | 124.40   |
| 9   | U1    | 75  | SER  | N-CA-C     | 9.07  | 119.88      | 107.73   |
| 3   | C1    | 115 | ILE  | CA-C-N     | -9.06 | 109.76      | 119.99   |
| 3   | C1    | 115 | ILE  | C-N-CA     | -9.06 | 109.76      | 119.99   |
| 2   | B1    | 42  | ALA  | CA-C-N     | 9.04  | 128.68      | 119.82   |
| 2   | B1    | 42  | ALA  | C-N-CA     | 9.04  | 128.68      | 119.82   |
| 5   | Q1    | 7   | VAL  | CA-C-N     | 9.04  | 129.11      | 119.89   |
| 5   | Q1    | 7   | VAL  | C-N-CA     | 9.04  | 129.11      | 119.89   |
| 2   | B1    | 178 | CYS  | CA-C-O     | -9.02 | 111.28      | 120.02   |
| 3   | O1    | 47  | THR  | CA-C-O     | 9.02  | 130.29      | 120.82   |
| 2   | B1    | 254 | HIS  | CA-CB-CG   | 8.98  | 122.78      | 113.80   |
| 63  | H3    | 52  | VAL  | N-CA-C     | 8.94  | 121.22      | 108.17   |
| 3   | O1    | 221 | HIS  | N-CA-CB    | 8.92  | 118.86      | 110.39   |
| 5   | Q1    | 166 | ASP  | CA-CB-CG   | 8.91  | 121.51      | 112.60   |
| 4   | D1    | 195 | GLU  | CA-C-N     | 8.83  | 129.72      | 119.47   |
| 4   | D1    | 195 | GLU  | C-N-CA     | 8.83  | 129.72      | 119.47   |
| 48  | f2    | 163 | LEU  | CA-C-N     | 8.82  | 148.18      | 127.00   |
| 48  | f2    | 163 | LEU  | C-N-CA     | 8.82  | 148.18      | 127.00   |
| 13  | 32    | 3   | LEU  | CA-C-N     | 8.82  | 137.57      | 121.70   |
| 13  | 32    | 3   | LEU  | C-N-CA     | 8.82  | 137.57      | 121.70   |
| 63  | H3    | 81  | PHE  | CA-C-N     | 8.77  | 128.42      | 119.56   |
| 63  | H3    | 81  | PHE  | C-N-CA     | 8.77  | 128.42      | 119.56   |
| 4   | D1    | 206 | LEU  | CB-CA-C    | -8.77 | 96.29       | 110.84   |
| 3   | C1    | 206 | ASN  | OD1-CG-ND2 | 8.74  | 131.34      | 122.60   |
| 1   | A1    | 256 | ALA  | N-CA-C     | 8.71  | 123.26      | 109.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | V1    | 14  | PHE  | CA-CB-CG    | 8.68  | 122.48      | 113.80   |
| 1   | A1    | 341 | GLN  | O-C-N       | 8.64  | 131.43      | 122.09   |
| 1   | M1    | 320 | LEU  | CA-C-O      | 8.63  | 130.02      | 120.70   |
| 3   | C1    | 196 | HIS  | O-C-N       | 8.63  | 131.01      | 122.03   |
| 3   | C1    | 43  | LEU  | O-C-N       | -8.61 | 112.80      | 122.09   |
| 5   | Q1    | 47  | VAL  | CA-C-O      | 8.59  | 129.99      | 121.05   |
| 3   | C1    | 175 | LEU  | N-CA-CB     | 8.53  | 123.44      | 110.30   |
| 5   | Q1    | 192 | MET  | CA-C-O      | 8.52  | 129.27      | 120.24   |
| 2   | B1    | 85  | ILE  | CB-CA-C     | -8.44 | 101.07      | 111.88   |
| 2   | B1    | 92  | VAL  | O-C-N       | -8.44 | 114.48      | 122.16   |
| 1   | A1    | 434 | TYR  | CA-C-O      | -8.42 | 111.53      | 120.63   |
| 5   | Q1    | 183 | PRO  | CA-C-O      | -8.42 | 110.19      | 122.31   |
| 3   | C1    | 182 | HIS  | CA-CB-CG    | 8.40  | 122.20      | 113.80   |
| 1   | A1    | 292 | SER  | CA-C-O      | 8.39  | 125.53      | 119.32   |
| 6   | F1    | 60  | PHE  | CA-CB-CG    | -8.37 | 105.43      | 113.80   |
| 3   | C1    | 246 | ALA  | N-CA-CB     | -8.32 | 101.30      | 110.71   |
| 3   | O1    | 242 | LEU  | CB-CA-C     | -8.28 | 98.12       | 110.95   |
| 7   | G1    | 13  | VAL  | O-C-N       | -8.27 | 114.32      | 123.26   |
| 2   | B1    | 369 | LEU  | CA-C-O      | 8.25  | 129.19      | 120.70   |
| 3   | O1    | 182 | HIS  | CA-CB-CG    | 8.22  | 122.02      | 113.80   |
| 6   | F1    | 43  | VAL  | CA-C-O      | 8.22  | 131.05      | 120.78   |
| 2   | B1    | 148 | LYS  | CA-C-N      | 8.21  | 131.11      | 120.44   |
| 2   | B1    | 148 | LYS  | C-N-CA      | 8.21  | 131.11      | 120.44   |
| 3   | O1    | 322 | GLN  | OE1-CD-NE2  | 8.21  | 130.81      | 122.60   |
| 5   | Q1    | 58  | PHE  | CA-CB-CG    | 8.18  | 121.98      | 113.80   |
| 6   | F1    | 64  | ARG  | CD-NE-CZ    | -8.14 | 113.01      | 124.40   |
| 6   | R1    | 63  | LYS  | CB-CA-C     | 8.14  | 123.66      | 110.88   |
| 5   | E1    | 60  | SER  | N-CA-C      | -8.13 | 103.36      | 113.28   |
| 67  | L3    | 20  | ARG  | N-CA-C      | -8.12 | 102.51      | 111.36   |
| 3   | C1    | 216 | ASP  | CA-CB-CG    | 8.12  | 120.72      | 112.60   |
| 1   | M1    | 419 | CYS  | CA-C-N      | 8.10  | 128.15      | 119.89   |
| 1   | M1    | 419 | CYS  | C-N-CA      | 8.10  | 128.15      | 119.89   |
| 56  | A3    | 82  | LEU  | N-CA-C      | 8.03  | 122.35      | 112.23   |
| 6   | F1    | 27  | ASN  | CA-C-O      | 8.02  | 129.49      | 120.90   |
| 1   | A1    | 294 | LEU  | O-C-N       | -8.02 | 113.62      | 122.12   |
| 2   | N1    | 141 | GLN  | OE1-CD-NE2  | -8.02 | 114.58      | 122.60   |
| 1   | A1    | 341 | GLN  | CA-C-O      | -7.99 | 112.47      | 120.70   |
| 3   | C1    | 43  | LEU  | CA-C-O      | 7.99  | 128.93      | 120.70   |
| 1   | M1    | 323 | HIS  | CA-CB-CG    | 7.99  | 121.79      | 113.80   |
| 5   | Q1    | 55  | VAL  | CA-CB-CG1   | 7.98  | 123.97      | 110.40   |
| 3   | C1    | 13  | ILE  | CB-CA-C     | -7.96 | 101.39      | 112.14   |
| 56  | A3    | 378 | HIS  | ND1-CE1-NE2 | 7.96  | 116.36      | 108.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | P1    | 202 | LYS  | CA-C-O     | -7.95 | 112.47      | 120.82   |
| 2   | N1    | 162 | ASN  | CA-CB-CG   | -7.95 | 104.65      | 112.60   |
| 1   | A1    | 431 | LEU  | CA-C-N     | 7.95  | 129.77      | 119.84   |
| 1   | A1    | 431 | LEU  | C-N-CA     | 7.95  | 129.77      | 119.84   |
| 2   | B1    | 320 | GLY  | O-C-N      | -7.93 | 117.84      | 123.95   |
| 1   | A1    | 168 | GLU  | O-C-N      | -7.90 | 112.97      | 122.22   |
| 5   | Q1    | 183 | PRO  | O-C-N      | 7.87  | 132.16      | 122.71   |
| 5   | Q1    | 135 | LEU  | O-C-N      | -7.85 | 113.58      | 123.24   |
| 3   | O1    | 257 | THR  | N-CA-CB    | 7.85  | 121.47      | 110.01   |
| 4   | D1    | 97  | ASN  | CA-C-N     | 7.85  | 129.65      | 119.84   |
| 4   | D1    | 97  | ASN  | C-N-CA     | 7.85  | 129.65      | 119.84   |
| 4   | P1    | 7   | PRO  | N-CA-C     | 7.83  | 120.26      | 110.70   |
| 5   | Q1    | 7   | VAL  | O-C-N      | 7.83  | 130.02      | 121.10   |
| 3   | C1    | 30  | TRP  | CA-C-O     | 7.82  | 129.07      | 120.63   |
| 2   | N1    | 412 | ASN  | OD1-CG-ND2 | 7.81  | 130.41      | 122.60   |
| 1   | M1    | 325 | VAL  | O-C-N      | -7.81 | 114.36      | 123.03   |
| 4   | D1    | 120 | ARG  | NE-CZ-NH2  | -7.80 | 112.18      | 119.20   |
| 3   | C1    | 33  | PHE  | CG-CD2-CE2 | 7.75  | 133.88      | 120.70   |
| 56  | A3    | 56  | VAL  | N-CA-C     | -7.74 | 103.25      | 110.53   |
| 3   | C1    | 321 | SER  | CA-C-N     | 7.72  | 131.40      | 120.28   |
| 3   | C1    | 321 | SER  | C-N-CA     | 7.72  | 131.40      | 120.28   |
| 1   | A1    | 438 | ARG  | NE-CZ-NH2  | 7.72  | 126.15      | 119.20   |
| 3   | O1    | 82  | MET  | CA-C-O     | 7.70  | 128.59      | 120.42   |
| 3   | C1    | 303 | LEU  | N-CA-CB    | 7.68  | 121.52      | 110.16   |
| 3   | C1    | 195 | VAL  | CA-C-O     | -7.67 | 112.97      | 120.95   |
| 5   | Q1    | 168 | SER  | N-CA-C     | -7.67 | 103.93      | 113.28   |
| 7   | S1    | 15  | THR  | CA-CB-CG2  | -7.67 | 97.47       | 110.50   |
| 56  | A3    | 435 | GLY  | N-CA-C     | 7.66  | 126.08      | 115.27   |
| 2   | B1    | 179 | PRO  | N-CA-CB    | 7.65  | 110.46      | 103.34   |
| 1   | M1    | 392 | LEU  | N-CA-C     | 7.64  | 120.28      | 111.11   |
| 3   | C1    | 185 | LEU  | CA-C-O     | 7.63  | 126.33      | 119.08   |
| 2   | N1    | 145 | ARG  | O-C-N      | 7.63  | 129.93      | 122.07   |
| 5   | Q1    | 56  | SER  | CA-C-O     | 7.62  | 128.82      | 120.82   |
| 1   | M1    | 420 | PRO  | N-CA-CB    | 7.62  | 109.72      | 103.32   |
| 3   | C1    | 123 | VAL  | CA-C-O     | 7.59  | 129.22      | 120.03   |
| 10  | V1    | 39  | ALA  | CA-C-O     | -7.59 | 112.50      | 120.55   |
| 1   | A1    | 242 | CYS  | CA-C-O     | 7.59  | 128.71      | 120.43   |
| 3   | O1    | 149 | LEU  | CA-C-O     | 7.58  | 128.91      | 119.05   |
| 3   | C1    | 85  | ASN  | CA-CB-CG   | -7.58 | 105.02      | 112.60   |
| 1   | A1    | 441 | MET  | CA-CB-CG   | -7.55 | 99.01       | 114.10   |
| 2   | B1    | 56  | ARG  | CD-NE-CZ   | 7.54  | 134.96      | 124.40   |
| 1   | A1    | 323 | HIS  | CA-CB-CG   | 7.53  | 121.33      | 113.80   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C1    | 273 | TYR  | CA-C-N    | -7.52 | 110.31      | 122.26   |
| 3   | C1    | 273 | TYR  | C-N-CA    | -7.52 | 110.31      | 122.26   |
| 3   | O1    | 242 | LEU  | N-CA-CB   | 7.51  | 120.88      | 109.98   |
| 41  | X2    | 43  | LEU  | CA-C-N    | 7.51  | 135.22      | 121.70   |
| 41  | X2    | 43  | LEU  | C-N-CA    | 7.51  | 135.22      | 121.70   |
| 1   | M1    | 434 | TYR  | O-C-N     | -7.50 | 114.30      | 122.09   |
| 1   | A1    | 244 | ARG  | NE-CZ-NH2 | 7.47  | 125.92      | 119.20   |
| 6   | R1    | 65  | ALA  | O-C-N     | -7.47 | 113.96      | 122.03   |
| 3   | C1    | 303 | LEU  | N-CA-C    | 7.46  | 119.50      | 111.36   |
| 7   | G1    | 26  | PHE  | CA-C-N    | 7.45  | 129.15      | 119.84   |
| 7   | G1    | 26  | PHE  | C-N-CA    | 7.45  | 129.15      | 119.84   |
| 3   | C1    | 106 | SER  | CA-C-O    | 7.45  | 128.58      | 119.79   |
| 3   | O1    | 71  | ARG  | NE-CZ-NH1 | -7.43 | 114.07      | 121.50   |
| 1   | M1    | 275 | ALA  | N-CA-C    | -7.41 | 103.14      | 111.07   |
| 4   | P1    | 235 | LEU  | O-C-N     | -7.41 | 113.56      | 123.19   |
| 3   | C1    | 205 | SER  | O-C-N     | -7.41 | 113.16      | 123.01   |
| 5   | Q1    | 179 | ASN  | CA-CB-CG  | 7.40  | 120.00      | 112.60   |
| 1   | M1    | 442 | PHE  | CA-CB-CG  | 7.37  | 121.17      | 113.80   |
| 56  | A3    | 330 | GLY  | N-CA-C    | 7.37  | 120.44      | 112.33   |
| 3   | O1    | 80  | ARG  | CD-NE-CZ  | -7.37 | 114.08      | 124.40   |
| 3   | C1    | 221 | HIS  | CA-CB-CG  | -7.36 | 106.44      | 113.80   |
| 7   | G1    | 13  | VAL  | CA-C-N    | -7.36 | 110.79      | 122.64   |
| 7   | G1    | 13  | VAL  | C-N-CA    | -7.36 | 110.79      | 122.64   |
| 68  | M3    | 27  | LEU  | N-CA-C    | 7.35  | 119.38      | 111.36   |
| 4   | D1    | 160 | MET  | N-CA-C    | 7.35  | 120.39      | 108.41   |
| 4   | D1    | 201 | ARG  | NE-CZ-NH1 | -7.35 | 114.15      | 121.50   |
| 1   | A1    | 364 | ALA  | O-C-N     | 7.34  | 129.90      | 122.12   |
| 3   | O1    | 222 | PRO  | CA-C-N    | 7.34  | 131.90      | 120.89   |
| 3   | O1    | 222 | PRO  | C-N-CA    | 7.34  | 131.90      | 120.89   |
| 3   | C1    | 313 | ARG  | NE-CZ-NH2 | 7.31  | 125.78      | 119.20   |
| 2   | B1    | 92  | VAL  | CA-C-O    | 7.30  | 127.02      | 119.35   |
| 3   | C1    | 195 | VAL  | O-C-N     | 7.30  | 128.95      | 121.87   |
| 3   | O1    | 88  | SER  | N-CA-C    | -7.26 | 103.30      | 111.07   |
| 1   | M1    | 256 | ALA  | CB-CA-C   | -7.26 | 93.45       | 109.56   |
| 3   | C1    | 30  | TRP  | O-C-N     | -7.25 | 114.43      | 122.12   |
| 1   | A1    | 281 | ASP  | CA-C-N    | 7.25  | 130.31      | 120.38   |
| 1   | A1    | 281 | ASP  | C-N-CA    | 7.25  | 130.31      | 120.38   |
| 2   | N1    | 188 | PRO  | O-C-N     | -7.25 | 112.85      | 122.64   |
| 1   | A1    | 435 | ASN  | CA-C-O    | 7.24  | 128.30      | 119.97   |
| 46  | c2    | 66  | ARG  | CA-C-N    | 7.24  | 134.73      | 121.70   |
| 46  | c2    | 66  | ARG  | C-N-CA    | 7.24  | 134.73      | 121.70   |
| 1   | M1    | 424 | GLY  | CA-C-O    | -7.24 | 113.59      | 121.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | N1    | 385 | GLN  | CA-C-O      | 7.23  | 128.09      | 120.42   |
| 5   | Q1    | 5   | ILE  | CB-CA-C     | -7.23 | 101.07      | 111.34   |
| 3   | C1    | 113 | TRP  | O-C-N       | -7.22 | 114.58      | 122.09   |
| 17  | 82    | 36  | LYS  | CA-C-N      | 7.22  | 134.69      | 121.70   |
| 17  | 82    | 36  | LYS  | C-N-CA      | 7.22  | 134.69      | 121.70   |
| 6   | F1    | 73  | GLN  | CB-CA-C     | 7.21  | 122.37      | 109.38   |
| 5   | Q1    | 72  | SER  | CA-C-O      | -7.21 | 113.26      | 121.19   |
| 56  | A3    | 376 | HIS  | CE1-NE2-CD2 | -7.21 | 101.79      | 109.00   |
| 1   | A1    | 419 | CYS  | N-CA-CB     | 7.20  | 119.66      | 110.23   |
| 56  | A3    | 9   | SER  | N-CA-C      | 7.19  | 119.84      | 110.43   |
| 4   | D1    | 215 | LEU  | CA-C-O      | 7.18  | 128.47      | 119.78   |
| 30  | L2    | 62  | ASN  | CA-C-N      | 7.16  | 134.60      | 121.70   |
| 30  | L2    | 62  | ASN  | C-N-CA      | 7.16  | 134.60      | 121.70   |
| 3   | C1    | 106 | SER  | N-CA-C      | -7.16 | 103.21      | 112.23   |
| 60  | E3    | 42  | VAL  | N-CA-C      | -7.15 | 99.61       | 108.05   |
| 17  | 82    | 228 | PRO  | CA-C-N      | 7.15  | 134.57      | 121.70   |
| 17  | 82    | 228 | PRO  | C-N-CA      | 7.15  | 134.57      | 121.70   |
| 4   | P1    | 199 | ASP  | CA-C-O      | -7.15 | 113.31      | 120.82   |
| 1   | M1    | 417 | ASP  | CA-C-N      | -7.15 | 109.73      | 122.74   |
| 1   | M1    | 417 | ASP  | C-N-CA      | -7.15 | 109.73      | 122.74   |
| 3   | O1    | 256 | TYR  | N-CA-C      | -7.13 | 104.51      | 112.57   |
| 3   | O1    | 37  | LEU  | CA-C-N      | 7.12  | 127.83      | 120.00   |
| 3   | O1    | 37  | LEU  | C-N-CA      | 7.12  | 127.83      | 120.00   |
| 5   | Q1    | 193 | VAL  | CG1-CB-CG2  | 7.12  | 126.47      | 110.80   |
| 1   | A1    | 242 | CYS  | O-C-N       | -7.12 | 115.23      | 123.27   |
| 3   | C1    | 264 | THR  | CB-CA-C     | -7.11 | 100.40      | 109.65   |
| 1   | A1    | 343 | MET  | CA-CB-CG    | -7.11 | 99.88       | 114.10   |
| 1   | M1    | 138 | LEU  | CA-C-O      | -7.11 | 112.70      | 121.02   |
| 56  | A3    | 332 | ILE  | N-CA-C      | 7.10  | 118.96      | 109.37   |
| 5   | E1    | 14  | ARG  | CA-C-N      | -7.10 | 113.73      | 123.96   |
| 5   | E1    | 14  | ARG  | C-N-CA      | -7.10 | 113.73      | 123.96   |
| 60  | E3    | 76  | GLY  | CA-C-N      | 7.10  | 128.33      | 120.45   |
| 60  | E3    | 76  | GLY  | C-N-CA      | 7.10  | 128.33      | 120.45   |
| 4   | D1    | 175 | THR  | CA-C-O      | 7.09  | 125.75      | 119.59   |
| 1   | M1    | 443 | TRP  | N-CA-C      | 7.08  | 121.70      | 107.41   |
| 3   | O1    | 244 | LEU  | O-C-N       | 7.07  | 131.57      | 122.10   |
| 7   | S1    | 21  | PHE  | CA-CB-CG    | -7.07 | 106.73      | 113.80   |
| 3   | O1    | 231 | GLY  | CA-C-O      | 7.06  | 128.07      | 120.30   |
| 17  | 82    | 259 | GLY  | CA-C-N      | 7.06  | 134.41      | 121.70   |
| 17  | 82    | 259 | GLY  | C-N-CA      | 7.06  | 134.41      | 121.70   |
| 5   | Q1    | 182 | VAL  | CA-C-O      | -7.04 | 116.09      | 120.88   |
| 6   | R1    | 60  | PHE  | CA-CB-CG    | -7.04 | 106.76      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B1    | 108 | THR  | N-CA-C      | 7.04  | 119.93      | 110.35   |
| 3   | C1    | 40  | CYS  | N-CA-C      | -7.04 | 103.36      | 112.23   |
| 2   | N1    | 291 | ALA  | N-CA-C      | -7.04 | 104.83      | 113.41   |
| 3   | O1    | 196 | HIS  | CE1-NE2-CD2 | -7.03 | 101.97      | 109.00   |
| 5   | Q1    | 135 | LEU  | CA-C-N      | 7.02  | 133.64      | 122.33   |
| 5   | Q1    | 135 | LEU  | C-N-CA      | 7.02  | 133.64      | 122.33   |
| 6   | R1    | 50  | LEU  | CA-C-N      | 7.02  | 128.62      | 119.84   |
| 6   | R1    | 50  | LEU  | C-N-CA      | 7.02  | 128.62      | 119.84   |
| 43  | Z2    | 85  | GLU  | CA-C-N      | 7.00  | 134.31      | 121.70   |
| 43  | Z2    | 85  | GLU  | C-N-CA      | 7.00  | 134.31      | 121.70   |
| 23  | E2    | 114 | ILE  | N-CA-C      | -7.00 | 106.48      | 113.20   |
| 1   | M1    | 414 | TYR  | N-CA-C      | 6.95  | 120.99      | 112.23   |
| 1   | A1    | 283 | THR  | N-CA-C      | 6.95  | 121.36      | 113.02   |
| 5   | Q1    | 25  | SER  | CA-C-O      | 6.94  | 127.06      | 119.15   |
| 58  | C3    | 36  | HIS  | N-CA-C      | 6.94  | 122.17      | 113.43   |
| 7   | G1    | 12  | HIS  | CA-C-N      | -6.93 | 114.06      | 123.14   |
| 7   | G1    | 12  | HIS  | C-N-CA      | -6.93 | 114.06      | 123.14   |
| 3   | C1    | 201 | HIS  | CA-CB-CG    | -6.93 | 106.87      | 113.80   |
| 2   | B1    | 97  | SER  | N-CA-C      | 6.92  | 120.95      | 109.46   |
| 4   | P1    | 83  | ARG  | CA-C-N      | 6.92  | 126.95      | 119.89   |
| 4   | P1    | 83  | ARG  | C-N-CA      | 6.92  | 126.95      | 119.89   |
| 6   | F1    | 45  | GLU  | CA-C-N      | -6.91 | 111.53      | 120.65   |
| 6   | F1    | 45  | GLU  | C-N-CA      | -6.91 | 111.53      | 120.65   |
| 56  | A3    | 130 | PRO  | N-CA-C      | -6.90 | 102.28      | 110.70   |
| 2   | N1    | 186 | VAL  | N-CA-CB     | 6.89  | 119.35      | 111.90   |
| 2   | N1    | 187 | THR  | N-CA-C      | 6.89  | 118.75      | 110.07   |
| 3   | O1    | 230 | LEU  | CA-C-N      | 6.89  | 128.97      | 120.22   |
| 3   | O1    | 230 | LEU  | C-N-CA      | 6.89  | 128.97      | 120.22   |
| 1   | A1    | 415 | PHE  | O-C-N       | -6.89 | 111.80      | 122.13   |
| 6   | F1    | 61  | ARG  | NE-CZ-NH2   | 6.87  | 125.39      | 119.20   |
| 5   | Q1    | 87  | MET  | CA-C-O      | 6.87  | 127.81      | 120.46   |
| 3   | O1    | 284 | ILE  | CA-C-O      | 6.86  | 123.65      | 119.19   |
| 2   | B1    | 70  | ARG  | NE-CZ-NH1   | -6.85 | 114.65      | 121.50   |
| 5   | Q1    | 14  | ARG  | NE-CZ-NH1   | -6.85 | 114.65      | 121.50   |
| 4   | P1    | 218 | LEU  | N-CA-CB     | 6.85  | 119.91      | 109.91   |
| 5   | E1    | 61  | SER  | CA-CB-OG    | -6.83 | 97.44       | 111.10   |
| 24  | F2    | 97  | MET  | C-N-CD      | -6.83 | 105.58      | 120.60   |
| 24  | F2    | 104 | ARG  | CA-C-N      | 6.83  | 133.99      | 121.70   |
| 24  | F2    | 104 | ARG  | C-N-CA      | 6.83  | 133.99      | 121.70   |
| 2   | B1    | 346 | THR  | CA-CB-OG1   | 6.82  | 119.83      | 109.60   |
| 3   | O1    | 241 | LEU  | O-C-N       | 6.82  | 129.93      | 122.15   |
| 3   | C1    | 135 | TRP  | CA-C-O      | -6.81 | 113.69      | 121.65   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | P1    | 97  | ASN  | CA-C-N     | 6.78  | 128.32      | 119.84   |
| 4   | P1    | 97  | ASN  | C-N-CA     | 6.78  | 128.32      | 119.84   |
| 19  | A2    | 461 | PRO  | CA-C-N     | 6.78  | 134.49      | 121.54   |
| 19  | A2    | 461 | PRO  | C-N-CA     | 6.78  | 134.49      | 121.54   |
| 1   | A1    | 338 | LEU  | CA-C-O     | 6.78  | 128.11      | 121.00   |
| 2   | B1    | 173 | ALA  | CA-C-O     | 6.77  | 127.99      | 119.12   |
| 2   | N1    | 258 | VAL  | N-CA-C     | 6.77  | 117.29      | 108.35   |
| 3   | O1    | 298 | ILE  | N-CA-C     | 6.77  | 116.89      | 110.53   |
| 10  | J1    | 14  | PHE  | CA-CB-CG   | 6.77  | 120.57      | 113.80   |
| 1   | M1    | 320 | LEU  | O-C-N      | -6.75 | 114.46      | 123.23   |
| 1   | M1    | 334 | MET  | N-CA-CB    | -6.75 | 100.17      | 110.16   |
| 5   | Q1    | 34  | GLY  | N-CA-C     | -6.75 | 104.33      | 112.49   |
| 3   | O1    | 13  | ILE  | CB-CA-C    | -6.74 | 103.20      | 112.02   |
| 59  | D3    | 133 | GLY  | N-CA-C     | 6.74  | 129.15      | 113.18   |
| 2   | N1    | 141 | GLN  | CA-C-N     | 6.73  | 128.25      | 119.84   |
| 2   | N1    | 141 | GLN  | C-N-CA     | 6.73  | 128.25      | 119.84   |
| 5   | Q1    | 194 | ILE  | N-CA-CB    | -6.73 | 103.43      | 111.90   |
| 1   | A1    | 436 | ARG  | O-C-N      | 6.72  | 129.35      | 122.09   |
| 56  | A3    | 507 | GLU  | N-CA-C     | -6.72 | 97.92       | 109.15   |
| 2   | B1    | 102 | ARG  | NE-CZ-NH2  | 6.71  | 125.24      | 119.20   |
| 3   | O1    | 328 | LEU  | CA-C-N     | -6.70 | 112.12      | 120.56   |
| 3   | O1    | 328 | LEU  | C-N-CA     | -6.70 | 112.12      | 120.56   |
| 62  | G3    | 5   | LYS  | N-CA-C     | 6.70  | 125.07      | 110.80   |
| 27  | I2    | 107 | THR  | CA-C-N     | -6.70 | 111.75      | 122.53   |
| 27  | I2    | 107 | THR  | C-N-CA     | -6.70 | 111.75      | 122.53   |
| 1   | A1    | 259 | GLY  | CA-C-N     | 6.69  | 128.21      | 119.84   |
| 1   | A1    | 259 | GLY  | C-N-CA     | 6.69  | 128.21      | 119.84   |
| 52  | I2    | 200 | LEU  | N-CA-C     | -6.69 | 104.82      | 114.12   |
| 3   | C1    | 109 | PHE  | CA-CB-CG   | 6.69  | 120.49      | 113.80   |
| 60  | E3    | 81  | ILE  | N-CA-C     | 6.69  | 116.82      | 110.53   |
| 5   | Q1    | 192 | MET  | N-CA-C     | 6.68  | 119.30      | 108.34   |
| 4   | D1    | 7   | PRO  | N-CA-C     | 6.68  | 118.85      | 110.70   |
| 2   | N1    | 173 | ALA  | CA-C-O     | 6.65  | 127.63      | 119.11   |
| 3   | C1    | 143 | ALA  | N-CA-C     | -6.65 | 104.11      | 111.36   |
| 1   | M1    | 334 | MET  | CA-C-O     | 6.65  | 127.47      | 120.42   |
| 3   | O1    | 222 | PRO  | CB-CA-C    | 6.64  | 122.52      | 111.56   |
| 6   | R1    | 35  | ASP  | CA-C-O     | 6.64  | 127.54      | 119.31   |
| 2   | B1    | 143 | GLN  | OE1-CD-NE2 | -6.64 | 115.96      | 122.60   |
| 3   | C1    | 218 | ILE  | O-C-N      | 6.62  | 128.65      | 121.10   |
| 5   | E1    | 14  | ARG  | CD-NE-CZ   | -6.62 | 115.13      | 124.40   |
| 3   | C1    | 186 | PRO  | O-C-N      | -6.61 | 114.64      | 122.24   |
| 4   | D1    | 32  | VAL  | N-CA-CB    | 6.60  | 117.84      | 110.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | Q1    | 129 | LYS  | CA-C-N     | 6.60  | 128.09      | 119.84   |
| 5   | Q1    | 129 | LYS  | C-N-CA     | 6.60  | 128.09      | 119.84   |
| 1   | M1    | 268 | VAL  | N-CA-C     | -6.60 | 106.36      | 112.96   |
| 56  | A3    | 61  | HIS  | CB-CG-CD2  | -6.60 | 122.62      | 131.20   |
| 3   | O1    | 19  | ILE  | CA-C-N     | 6.60  | 134.33      | 122.06   |
| 3   | O1    | 19  | ILE  | C-N-CA     | 6.60  | 134.33      | 122.06   |
| 1   | A1    | 169 | GLY  | CA-C-N     | 6.59  | 128.08      | 119.84   |
| 1   | A1    | 169 | GLY  | C-N-CA     | 6.59  | 128.08      | 119.84   |
| 2   | B1    | 177 | TYR  | CA-C-O     | -6.58 | 113.20      | 120.38   |
| 56  | A3    | 506 | GLU  | N-CA-C     | -6.57 | 104.11      | 111.28   |
| 4   | D1    | 92  | PRO  | N-CA-CB    | 6.57  | 107.63      | 103.23   |
| 3   | O1    | 299 | LEU  | CA-C-O     | 6.56  | 127.43      | 119.49   |
| 9   | I1    | 68  | VAL  | CB-CA-C    | -6.56 | 101.74      | 110.98   |
| 1   | A1    | 331 | ILE  | N-CA-C     | 6.55  | 117.24      | 110.36   |
| 38  | U2    | 120 | THR  | CA-C-N     | 6.55  | 142.73      | 127.00   |
| 38  | U2    | 120 | THR  | C-N-CA     | 6.55  | 142.73      | 127.00   |
| 2   | N1    | 62  | ASN  | CA-CB-CG   | 6.55  | 119.15      | 112.60   |
| 1   | A1    | 436 | ARG  | N-CA-CB    | 6.55  | 119.57      | 110.07   |
| 2   | B1    | 75  | LEU  | CA-C-O     | -6.54 | 114.42      | 121.94   |
| 6   | R1    | 79  | GLN  | N-CA-C     | 6.54  | 120.26      | 112.93   |
| 56  | A3    | 74  | MET  | N-CA-C     | 6.54  | 118.07      | 111.07   |
| 1   | A1    | 189 | HIS  | CA-CB-CG   | 6.54  | 120.34      | 113.80   |
| 3   | O1    | 93  | CYS  | N-CA-CB    | 6.54  | 119.84      | 110.16   |
| 5   | Q1    | 24  | SER  | N-CA-C     | 6.54  | 119.71      | 110.23   |
| 8   | H1    | 67  | HIS  | CA-CB-CG   | 6.54  | 120.33      | 113.80   |
| 3   | C1    | 246 | ALA  | O-C-N      | 6.53  | 125.96      | 121.19   |
| 3   | O1    | 244 | LEU  | CA-C-O     | -6.53 | 111.87      | 119.64   |
| 5   | Q1    | 70  | ALA  | CA-C-O     | 6.53  | 127.34      | 120.42   |
| 44  | a2    | 128 | SER  | CA-C-N     | 6.52  | 133.44      | 121.70   |
| 44  | a2    | 128 | SER  | C-N-CA     | 6.52  | 133.44      | 121.70   |
| 11  | K1    | 35  | ALA  | N-CA-C     | -6.51 | 104.10      | 111.07   |
| 4   | D1    | 229 | VAL  | CB-CA-C    | -6.51 | 103.63      | 111.97   |
| 3   | C1    | 312 | GLN  | O-C-N      | -6.51 | 114.69      | 122.63   |
| 3   | C1    | 322 | GLN  | OE1-CD-NE2 | 6.50  | 129.10      | 122.60   |
| 4   | D1    | 83  | ARG  | CA-C-N     | 6.50  | 126.52      | 119.89   |
| 4   | D1    | 83  | ARG  | C-N-CA     | 6.50  | 126.52      | 119.89   |
| 1   | M1    | 307 | PHE  | O-C-N      | -6.50 | 115.44      | 123.44   |
| 1   | A1    | 199 | ALA  | CA-C-N     | -6.50 | 112.39      | 122.59   |
| 1   | A1    | 199 | ALA  | C-N-CA     | -6.50 | 112.39      | 122.59   |
| 2   | B1    | 187 | THR  | CA-C-N     | 6.49  | 127.95      | 119.84   |
| 2   | B1    | 187 | THR  | C-N-CA     | 6.49  | 127.95      | 119.84   |
| 2   | B1    | 29  | LEU  | CA-C-N     | 6.48  | 126.24      | 119.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B1    | 29  | LEU  | C-N-CA      | 6.48  | 126.24      | 119.05   |
| 3   | C1    | 230 | LEU  | CA-C-N      | 6.48  | 127.31      | 119.99   |
| 3   | C1    | 230 | LEU  | C-N-CA      | 6.48  | 127.31      | 119.99   |
| 2   | B1    | 91  | ALA  | CA-C-N      | 6.48  | 132.34      | 122.69   |
| 2   | B1    | 91  | ALA  | C-N-CA      | 6.48  | 132.34      | 122.69   |
| 5   | E1    | 6   | LYS  | O-C-N       | -6.47 | 115.37      | 123.27   |
| 56  | A3    | 61  | HIS  | ND1-CE1-NE2 | 6.46  | 114.86      | 108.40   |
| 1   | A1    | 438 | ARG  | NE-CZ-NH1   | -6.46 | 115.05      | 121.50   |
| 3   | C1    | 224 | TYR  | N-CA-C      | 6.45  | 120.41      | 112.54   |
| 1   | A1    | 435 | ASN  | OD1-CG-ND2  | 6.45  | 129.05      | 122.60   |
| 7   | S1    | 26  | PHE  | CA-C-N      | 6.45  | 127.90      | 119.84   |
| 7   | S1    | 26  | PHE  | C-N-CA      | 6.45  | 127.90      | 119.84   |
| 1   | M1    | 100 | LYS  | CA-C-O      | -6.45 | 113.40      | 120.43   |
| 3   | O1    | 80  | ARG  | NE-CZ-NH1   | -6.44 | 115.06      | 121.50   |
| 3   | C1    | 293 | ALA  | CA-C-N      | -6.43 | 111.16      | 120.29   |
| 3   | C1    | 293 | ALA  | C-N-CA      | -6.43 | 111.16      | 120.29   |
| 6   | R1    | 36  | THR  | CA-CB-CG2   | 6.43  | 121.43      | 110.50   |
| 1   | M1    | 174 | VAL  | CA-CB-CG1   | 6.43  | 121.33      | 110.40   |
| 1   | A1    | 280 | TYR  | O-C-N       | -6.42 | 116.07      | 123.33   |
| 5   | E1    | 5   | ILE  | CB-CA-C     | -6.42 | 102.42      | 111.21   |
| 1   | A1    | 420 | PRO  | N-CA-CB     | 6.40  | 109.41      | 103.39   |
| 3   | C1    | 109 | PHE  | O-C-N       | -6.40 | 114.07      | 122.59   |
| 5   | Q1    | 29  | SER  | N-CA-C      | 6.40  | 120.81      | 113.19   |
| 7   | G1    | 4   | PHE  | CA-CB-CG    | -6.39 | 107.41      | 113.80   |
| 2   | N1    | 178 | CYS  | CA-C-N      | 6.38  | 126.14      | 119.76   |
| 2   | N1    | 178 | CYS  | C-N-CA      | 6.38  | 126.14      | 119.76   |
| 2   | N1    | 204 | MET  | N-CA-C      | 6.38  | 120.45      | 110.17   |
| 3   | C1    | 107 | TYR  | CA-C-N      | -6.38 | 111.64      | 120.38   |
| 3   | C1    | 107 | TYR  | C-N-CA      | -6.38 | 111.64      | 120.38   |
| 1   | A1    | 436 | ARG  | CA-C-O      | -6.38 | 114.13      | 120.70   |
| 1   | M1    | 150 | PHE  | CA-CB-CG    | 6.38  | 120.18      | 113.80   |
| 1   | A1    | 147 | ASP  | CA-C-O      | 6.37  | 127.31      | 120.24   |
| 23  | E2    | 75  | SER  | CA-C-N      | 6.36  | 133.14      | 121.70   |
| 23  | E2    | 75  | SER  | C-N-CA      | 6.36  | 133.14      | 121.70   |
| 3   | O1    | 256 | TYR  | O-C-N       | 6.35  | 130.39      | 122.19   |
| 6   | F1    | 14  | GLU  | CA-C-N      | 6.34  | 126.97      | 120.00   |
| 6   | F1    | 14  | GLU  | C-N-CA      | 6.34  | 126.97      | 120.00   |
| 38  | U2    | 120 | THR  | C-N-CD      | -6.34 | 106.66      | 120.60   |
| 1   | A1    | 11  | VAL  | CA-C-N      | 6.33  | 127.76      | 119.84   |
| 1   | A1    | 11  | VAL  | C-N-CA      | 6.33  | 127.76      | 119.84   |
| 1   | M1    | 239 | SER  | CA-C-O      | -6.33 | 114.24      | 121.58   |
| 55  | e2    | 70  | THR  | N-CA-C      | 6.32  | 117.35      | 108.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A1    | 24  | ARG  | NE-CZ-NH1 | -6.32 | 115.18      | 121.50   |
| 4   | D1    | 168 | VAL  | CB-CA-C   | -6.31 | 103.78      | 112.24   |
| 1   | A1    | 32  | GLN  | CA-C-N    | 6.31  | 127.73      | 119.84   |
| 1   | A1    | 32  | GLN  | C-N-CA    | 6.31  | 127.73      | 119.84   |
| 1   | A1    | 251 | ALA  | CA-C-N    | -6.31 | 114.38      | 122.77   |
| 1   | A1    | 251 | ALA  | C-N-CA    | -6.31 | 114.38      | 122.77   |
| 3   | C1    | 301 | LEU  | N-CA-C    | 6.31  | 118.68      | 111.11   |
| 1   | A1    | 150 | PHE  | CA-CB-CG  | 6.31  | 120.11      | 113.80   |
| 3   | O1    | 325 | PHE  | O-C-N     | 6.30  | 128.58      | 122.03   |
| 2   | B1    | 73  | SER  | CA-C-O    | -6.29 | 111.52      | 120.51   |
| 2   | B1    | 89  | ILE  | CA-CB-CG2 | 6.29  | 121.18      | 110.50   |
| 36  | S2    | 113 | ASP  | CA-C-N    | 6.28  | 133.01      | 121.70   |
| 36  | S2    | 113 | ASP  | C-N-CA    | 6.28  | 133.01      | 121.70   |
| 2   | B1    | 145 | ARG  | CA-C-O    | -6.28 | 114.18      | 120.90   |
| 6   | R1    | 24  | ALA  | CA-C-O    | 6.28  | 129.49      | 120.51   |
| 2   | N1    | 254 | HIS  | CA-C-O    | -6.27 | 113.93      | 120.70   |
| 2   | B1    | 291 | ALA  | N-CA-C    | -6.27 | 105.76      | 113.41   |
| 56  | A3    | 10  | THR  | N-CA-C    | -6.25 | 103.84      | 112.03   |
| 12  | 22    | 141 | VAL  | N-CA-C    | -6.25 | 106.87      | 112.12   |
| 5   | Q1    | 123 | ASP  | CA-CB-CG  | -6.25 | 106.35      | 112.60   |
| 1   | M1    | 319 | LEU  | N-CA-CB   | -6.25 | 100.74      | 110.55   |
| 3   | C1    | 78  | ILE  | CA-C-N    | -6.24 | 111.55      | 120.42   |
| 3   | C1    | 78  | ILE  | C-N-CA    | -6.24 | 111.55      | 120.42   |
| 35  | R2    | 271 | TYR  | CA-C-N    | 6.24  | 133.47      | 121.54   |
| 35  | R2    | 271 | TYR  | C-N-CA    | 6.24  | 133.47      | 121.54   |
| 1   | A1    | 434 | TYR  | O-C-N     | 6.23  | 128.72      | 122.12   |
| 62  | G3    | 2   | SER  | N-CA-C    | 6.23  | 119.51      | 109.79   |
| 1   | A1    | 196 | VAL  | CA-C-O    | -6.22 | 113.91      | 120.76   |
| 5   | Q1    | 14  | ARG  | CD-NE-CZ  | -6.22 | 115.69      | 124.40   |
| 4   | P1    | 110 | PRO  | CA-C-N    | 6.22  | 126.17      | 119.76   |
| 4   | P1    | 110 | PRO  | C-N-CA    | 6.22  | 126.17      | 119.76   |
| 7   | G1    | 14  | ILE  | CA-C-N    | 6.22  | 131.95      | 122.93   |
| 7   | G1    | 14  | ILE  | C-N-CA    | 6.22  | 131.95      | 122.93   |
| 1   | M1    | 342 | TRP  | CA-C-N    | 6.22  | 128.93      | 120.54   |
| 1   | M1    | 342 | TRP  | C-N-CA    | 6.22  | 128.93      | 120.54   |
| 60  | E3    | 21  | LYS  | CA-C-N    | 6.21  | 126.40      | 119.32   |
| 60  | E3    | 21  | LYS  | C-N-CA    | 6.21  | 126.40      | 119.32   |
| 1   | A1    | 69  | ASN  | O-C-N     | -6.21 | 115.58      | 122.03   |
| 2   | N1    | 167 | ALA  | CA-C-O    | 6.21  | 127.11      | 119.97   |
| 1   | M1    | 277 | ILE  | CA-C-O    | -6.20 | 114.82      | 121.27   |
| 7   | S1    | 58  | VAL  | N-CA-CB   | 6.20  | 117.39      | 110.51   |
| 7   | G1    | 21  | PHE  | CA-CB-CG  | -6.20 | 107.60      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M1    | 416 | TYR  | N-CA-C      | 6.19  | 118.27      | 108.67   |
| 1   | A1    | 343 | MET  | CA-C-N      | -6.19 | 111.90      | 120.38   |
| 1   | A1    | 343 | MET  | C-N-CA      | -6.19 | 111.90      | 120.38   |
| 5   | Q1    | 153 | PHE  | CA-CB-CG    | 6.18  | 119.98      | 113.80   |
| 5   | Q1    | 66  | ALA  | CA-C-O      | 6.18  | 127.22      | 119.12   |
| 1   | A1    | 392 | LEU  | N-CA-CB     | 6.18  | 119.14      | 109.94   |
| 1   | M1    | 161 | THR  | CA-C-N      | 6.18  | 126.64      | 119.47   |
| 1   | M1    | 161 | THR  | C-N-CA      | 6.18  | 126.64      | 119.47   |
| 7   | S1    | 34  | ILE  | CA-C-N      | 6.17  | 125.66      | 119.24   |
| 7   | S1    | 34  | ILE  | C-N-CA      | 6.17  | 125.66      | 119.24   |
| 5   | E1    | 29  | SER  | N-CA-C      | 6.17  | 120.27      | 112.87   |
| 10  | J1    | 8   | ARG  | CA-C-N      | 6.17  | 128.87      | 120.54   |
| 10  | J1    | 8   | ARG  | C-N-CA      | 6.17  | 128.87      | 120.54   |
| 51  | j2    | 22  | PRO  | CA-C-N      | 6.16  | 141.79      | 127.00   |
| 51  | j2    | 22  | PRO  | C-N-CA      | 6.16  | 141.79      | 127.00   |
| 3   | C1    | 231 | GLY  | CA-C-O      | 6.15  | 127.38      | 121.05   |
| 1   | M1    | 142 | ASP  | N-CA-C      | -6.15 | 105.74      | 113.18   |
| 1   | A1    | 408 | ARG  | NH1-CZ-NH2  | 6.14  | 127.28      | 119.30   |
| 6   | R1    | 98  | ILE  | CA-C-O      | 6.13  | 127.65      | 121.27   |
| 1   | A1    | 440 | GLY  | CA-C-N      | -6.13 | 112.01      | 122.56   |
| 1   | A1    | 440 | GLY  | C-N-CA      | -6.13 | 112.01      | 122.56   |
| 4   | P1    | 160 | MET  | N-CA-C      | 6.13  | 118.74      | 108.02   |
| 2   | N1    | 66  | SER  | N-CA-CB     | 6.12  | 118.88      | 110.01   |
| 1   | A1    | 338 | LEU  | O-C-N       | -6.12 | 115.67      | 122.03   |
| 2   | B1    | 46  | ARG  | N-CA-C      | 6.10  | 118.36      | 107.80   |
| 2   | B1    | 306 | PRO  | N-CA-CB     | 6.10  | 108.18      | 103.30   |
| 3   | C1    | 180 | ALA  | N-CA-CB     | 6.10  | 119.16      | 110.13   |
| 6   | R1    | 58  | ARG  | NE-CZ-NH2   | 6.10  | 124.69      | 119.20   |
| 3   | O1    | 233 | LEU  | O-C-N       | 6.09  | 128.43      | 122.09   |
| 16  | 72    | 140 | ALA  | CA-C-N      | 6.09  | 132.67      | 121.70   |
| 16  | 72    | 140 | ALA  | C-N-CA      | 6.09  | 132.67      | 121.70   |
| 2   | N1    | 412 | ASN  | CB-CG-ND2   | -6.07 | 107.29      | 116.40   |
| 7   | S1    | 10  | VAL  | CA-C-O      | -6.07 | 114.14      | 120.27   |
| 3   | C1    | 13  | ILE  | CA-CB-CG1   | 6.07  | 120.72      | 110.40   |
| 3   | O1    | 196 | HIS  | ND1-CE1-NE2 | 6.07  | 114.47      | 108.40   |
| 1   | A1    | 153 | LEU  | N-CA-CB     | 6.07  | 119.04      | 109.82   |
| 1   | A1    | 418 | GLN  | CA-C-N      | -6.07 | 113.18      | 121.61   |
| 1   | A1    | 418 | GLN  | C-N-CA      | -6.07 | 113.18      | 121.61   |
| 36  | S2    | 87  | GLY  | CA-C-N      | 6.07  | 132.62      | 121.70   |
| 36  | S2    | 87  | GLY  | C-N-CA      | 6.07  | 132.62      | 121.70   |
| 3   | O1    | 221 | HIS  | CB-CA-C     | -6.06 | 104.05      | 113.57   |
| 56  | A3    | 157 | SER  | N-CA-C      | 6.06  | 118.85      | 111.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 56  | A3    | 170 | ASN  | N-CA-C     | 6.06  | 120.75      | 113.23   |
| 5   | E1    | 32  | ARG  | NE-CZ-NH1  | -6.06 | 115.44      | 121.50   |
| 1   | M1    | 292 | SER  | CA-C-N     | 6.06  | 127.41      | 119.84   |
| 1   | M1    | 292 | SER  | C-N-CA     | 6.06  | 127.41      | 119.84   |
| 2   | N1    | 87  | ARG  | O-C-N      | 6.06  | 129.31      | 122.22   |
| 3   | C1    | 280 | ILE  | N-CA-CB    | 6.04  | 118.02      | 110.47   |
| 16  | 72    | 109 | LYS  | N-CA-C     | -6.04 | 107.74      | 114.62   |
| 1   | A1    | 277 | ILE  | CB-CA-C    | -6.03 | 104.00      | 112.14   |
| 1   | A1    | 292 | SER  | O-C-N      | -6.03 | 115.80      | 121.35   |
| 19  | A2    | 381 | LEU  | CA-C-N     | 6.02  | 133.04      | 121.54   |
| 19  | A2    | 381 | LEU  | C-N-CA     | 6.02  | 133.04      | 121.54   |
| 3   | C1    | 186 | PRO  | CA-C-O     | 6.01  | 130.00      | 119.84   |
| 3   | O1    | 320 | LEU  | CA-C-N     | -6.01 | 111.17      | 120.31   |
| 3   | O1    | 320 | LEU  | C-N-CA     | -6.01 | 111.17      | 120.31   |
| 1   | M1    | 205 | HIS  | CA-CB-CG   | -6.01 | 107.79      | 113.80   |
| 2   | N1    | 85  | ILE  | O-C-N      | 6.01  | 130.08      | 122.57   |
| 2   | B1    | 409 | ASP  | CA-C-N     | 6.01  | 128.64      | 120.77   |
| 2   | B1    | 409 | ASP  | C-N-CA     | 6.01  | 128.64      | 120.77   |
| 2   | B1    | 187 | THR  | CA-C-O     | -6.00 | 115.20      | 120.60   |
| 56  | A3    | 125 | GLY  | N-CA-C     | -6.00 | 104.14      | 112.18   |
| 63  | H3    | 63  | LEU  | N-CA-C     | 6.00  | 119.07      | 111.69   |
| 1   | M1    | 54  | GLY  | O-C-N      | 6.00  | 127.67      | 121.97   |
| 2   | N1    | 306 | PRO  | N-CA-CB    | 6.00  | 108.10      | 103.30   |
| 4   | D1    | 86  | LYS  | N-CA-C     | 6.00  | 118.51      | 110.35   |
| 3   | C1    | 19  | ILE  | CA-C-O     | -6.00 | 113.82      | 120.96   |
| 47  | d2    | 31  | PHE  | CA-C-N     | 5.99  | 141.38      | 127.00   |
| 47  | d2    | 31  | PHE  | C-N-CA     | 5.99  | 141.38      | 127.00   |
| 25  | G2    | 155 | PRO  | CA-C-N     | 5.99  | 132.48      | 121.70   |
| 25  | G2    | 155 | PRO  | C-N-CA     | 5.99  | 132.48      | 121.70   |
| 3   | C1    | 179 | PHE  | CA-CB-CG   | 5.98  | 119.78      | 113.80   |
| 1   | M1    | 274 | ASN  | OD1-CG-ND2 | 5.98  | 128.58      | 122.60   |
| 57  | B3    | 207 | MET  | CA-C-N     | 5.98  | 127.31      | 119.84   |
| 57  | B3    | 207 | MET  | C-N-CA     | 5.98  | 127.31      | 119.84   |
| 57  | B3    | 47  | THR  | N-CA-C     | 5.98  | 119.88      | 112.59   |
| 58  | C3    | 8   | TYR  | N-CA-C     | 5.98  | 118.24      | 110.53   |
| 3   | O1    | 102 | LEU  | O-C-N      | 5.98  | 130.71      | 122.46   |
| 3   | C1    | 143 | ALA  | CA-C-O     | 5.97  | 126.75      | 120.42   |
| 7   | S1    | 50  | PRO  | N-CA-C     | 5.97  | 117.98      | 110.70   |
| 1   | M1    | 438 | ARG  | CA-CB-CG   | -5.97 | 102.17      | 114.10   |
| 7   | S1    | 4   | PHE  | CA-CB-CG   | -5.97 | 107.83      | 113.80   |
| 1   | A1    | 425 | PHE  | N-CA-CB    | 5.96  | 121.11      | 110.79   |
| 2   | B1    | 102 | ARG  | NE-CZ-NH1  | -5.96 | 115.54      | 121.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M1    | 342 | TRP  | CH2-CZ2-CE2 | 5.96  | 125.25      | 117.50   |
| 1   | M1    | 416 | TYR  | CA-C-O      | -5.96 | 113.86      | 120.60   |
| 8   | H1    | 55  | THR  | CA-C-O      | 5.96  | 127.08      | 120.82   |
| 33  | P2    | 51  | ASN  | N-CA-C      | -5.96 | 107.82      | 114.62   |
| 62  | G3    | 44  | ARG  | CA-C-N      | 5.96  | 125.98      | 119.90   |
| 62  | G3    | 44  | ARG  | C-N-CA      | 5.96  | 125.98      | 119.90   |
| 1   | A1    | 166 | SER  | CA-C-O      | 5.96  | 127.83      | 121.16   |
| 5   | Q1    | 80  | ASP  | CA-CB-CG    | -5.95 | 106.65      | 112.60   |
| 1   | A1    | 440 | GLY  | N-CA-C      | -5.95 | 107.52      | 115.32   |
| 3   | C1    | 257 | THR  | CA-C-O      | 5.94  | 123.72      | 119.32   |
| 1   | A1    | 284 | TYR  | O-C-N       | -5.93 | 115.63      | 122.93   |
| 2   | B1    | 145 | ARG  | O-C-N       | 5.93  | 128.26      | 122.09   |
| 3   | O1    | 210 | GLY  | N-CA-C      | -5.93 | 107.21      | 114.92   |
| 5   | Q1    | 99  | ARG  | NE-CZ-NH2   | 5.93  | 124.54      | 119.20   |
| 1   | M1    | 89  | TYR  | CA-CB-CG    | 5.93  | 124.57      | 113.90   |
| 2   | N1    | 75  | LEU  | N-CA-CB     | 5.93  | 118.92      | 110.44   |
| 1   | A1    | 248 | LEU  | CA-C-N      | 5.92  | 125.80      | 119.28   |
| 1   | A1    | 248 | LEU  | C-N-CA      | 5.92  | 125.80      | 119.28   |
| 2   | N1    | 143 | GLN  | OE1-CD-NE2  | -5.92 | 116.68      | 122.60   |
| 5   | Q1    | 132 | TRP  | N-CA-C      | 5.92  | 119.46      | 109.76   |
| 12  | 22    | 127 | GLY  | CA-C-N      | 5.92  | 132.35      | 121.70   |
| 12  | 22    | 127 | GLY  | C-N-CA      | 5.92  | 132.35      | 121.70   |
| 4   | D1    | 110 | PRO  | CA-C-N      | 5.91  | 125.85      | 119.76   |
| 4   | D1    | 110 | PRO  | C-N-CA      | 5.91  | 125.85      | 119.76   |
| 3   | C1    | 22  | PRO  | CB-CA-C     | -5.91 | 101.80      | 111.56   |
| 10  | J1    | 22  | LEU  | N-CA-C      | -5.91 | 104.75      | 111.07   |
| 4   | P1    | 138 | PRO  | N-CD-CG     | -5.91 | 94.33       | 103.20   |
| 56  | A3    | 67  | PHE  | N-CA-C      | 5.91  | 119.68      | 112.23   |
| 3   | C1    | 127 | ALA  | CA-C-O      | 5.91  | 126.76      | 119.97   |
| 44  | a2    | 19  | ASP  | CA-C-N      | 5.90  | 141.17      | 127.00   |
| 44  | a2    | 19  | ASP  | C-N-CA      | 5.90  | 141.17      | 127.00   |
| 56  | A3    | 171 | MET  | N-CA-C      | 5.90  | 120.19      | 111.87   |
| 1   | M1    | 46  | ARG  | NH1-CZ-NH2  | 5.90  | 126.97      | 119.30   |
| 3   | C1    | 71  | ARG  | NE-CZ-NH1   | -5.89 | 115.61      | 121.50   |
| 4   | D1    | 92  | PRO  | CB-CA-C     | 5.89  | 116.76      | 111.40   |
| 3   | C1    | 91  | PHE  | CB-CG-CD2   | -5.89 | 110.69      | 120.70   |
| 3   | C1    | 160 | LEU  | N-CA-C      | 5.89  | 118.46      | 111.33   |
| 2   | N1    | 167 | ALA  | O-C-N       | -5.89 | 115.02      | 122.27   |
| 3   | O1    | 126 | THR  | O-C-N       | 5.89  | 128.14      | 122.07   |
| 56  | A3    | 119 | GLU  | CB-CA-C     | -5.89 | 109.77      | 116.54   |
| 7   | S1    | 15  | THR  | CB-CA-C     | -5.88 | 98.94       | 109.71   |
| 57  | B3    | 134 | ARG  | N-CA-C      | 5.88  | 123.33      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C1    | 282 | ARG  | CD-NE-CZ   | -5.87 | 116.18      | 124.40   |
| 3   | C1    | 176 | THR  | CA-CB-OG1  | -5.87 | 100.79      | 109.60   |
| 3   | C1    | 320 | LEU  | CA-C-N     | -5.87 | 111.39      | 120.31   |
| 3   | C1    | 320 | LEU  | C-N-CA     | -5.87 | 111.39      | 120.31   |
| 2   | N1    | 285 | VAL  | N-CA-C     | 5.87  | 116.73      | 108.17   |
| 1   | A1    | 281 | ASP  | CA-CB-CG   | 5.85  | 118.45      | 112.60   |
| 3   | C1    | 177 | ARG  | CB-CA-C    | -5.85 | 101.95      | 110.96   |
| 2   | N1    | 42  | ALA  | CA-C-N     | 5.85  | 127.15      | 119.84   |
| 2   | N1    | 42  | ALA  | C-N-CA     | 5.85  | 127.15      | 119.84   |
| 2   | N1    | 157 | ALA  | N-CA-C     | 5.85  | 117.33      | 111.07   |
| 5   | E1    | 15  | ARG  | O-C-N      | 5.85  | 126.29      | 121.32   |
| 1   | M1    | 364 | ALA  | CA-C-O     | 5.85  | 126.75      | 120.55   |
| 16  | 72    | 139 | GLU  | CA-C-N     | 5.85  | 132.22      | 121.70   |
| 16  | 72    | 139 | GLU  | C-N-CA     | 5.85  | 132.22      | 121.70   |
| 3   | O1    | 206 | ASN  | O-C-N      | -5.84 | 115.78      | 122.68   |
| 3   | C1    | 205 | SER  | CA-C-O     | 5.84  | 127.42      | 120.70   |
| 2   | N1    | 47  | ILE  | CB-CG1-CD1 | 5.84  | 126.07      | 113.80   |
| 2   | N1    | 157 | ALA  | N-CA-CB    | 5.84  | 118.48      | 110.01   |
| 3   | O1    | 227 | LYS  | O-C-N      | 5.84  | 128.08      | 122.07   |
| 3   | C1    | 282 | ARG  | NE-CZ-NH1  | -5.83 | 115.67      | 121.50   |
| 3   | O1    | 50  | PHE  | CA-CB-CG   | -5.83 | 107.97      | 113.80   |
| 1   | A1    | 311 | ASN  | OD1-CG-ND2 | 5.82  | 128.42      | 122.60   |
| 2   | B1    | 245 | ARG  | NE-CZ-NH1  | -5.82 | 115.68      | 121.50   |
| 2   | B1    | 94  | GLY  | CA-C-O     | -5.82 | 114.31      | 122.51   |
| 2   | N1    | 85  | ILE  | CA-C-O     | -5.81 | 113.51      | 120.78   |
| 3   | O1    | 280 | ILE  | CB-CG1-CD1 | 5.81  | 126.01      | 113.80   |
| 4   | P1    | 229 | VAL  | N-CA-CB    | 5.81  | 116.96      | 110.51   |
| 2   | B1    | 138 | ALA  | CA-C-O     | -5.81 | 114.26      | 120.42   |
| 4   | D1    | 182 | VAL  | N-CA-CB    | 5.81  | 119.29      | 110.58   |
| 55  | e2    | 94  | HIS  | N-CA-C     | 5.80  | 122.63      | 109.81   |
| 1   | A1    | 352 | SER  | CA-CB-OG   | 5.80  | 122.69      | 111.10   |
| 4   | D1    | 151 | PRO  | N-CA-CB    | 5.79  | 108.85      | 103.41   |
| 2   | N1    | 167 | ALA  | CA-C-N     | -5.79 | 112.39      | 122.64   |
| 2   | N1    | 167 | ALA  | C-N-CA     | -5.79 | 112.39      | 122.64   |
| 14  | 42    | 457 | PRO  | CA-C-N     | 5.79  | 132.12      | 121.70   |
| 14  | 42    | 457 | PRO  | C-N-CA     | 5.79  | 132.12      | 121.70   |
| 5   | Q1    | 18  | VAL  | CB-CA-C    | -5.78 | 101.81      | 111.29   |
| 3   | O1    | 201 | HIS  | CA-C-O     | 5.77  | 126.05      | 119.18   |
| 3   | C1    | 189 | ILE  | CB-CA-C    | -5.77 | 104.48      | 112.04   |
| 19  | A2    | 504 | SER  | CA-C-N     | 5.76  | 132.08      | 121.70   |
| 19  | A2    | 504 | SER  | C-N-CA     | 5.76  | 132.08      | 121.70   |
| 3   | C1    | 75  | TYR  | N-CA-C     | -5.76 | 106.20      | 113.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | O1    | 38  | GLY  | O-C-N      | -5.76 | 116.60      | 122.19   |
| 58  | C3    | 198 | PHE  | N-CA-C     | 5.76  | 117.56      | 111.28   |
| 6   | R1    | 28  | LYS  | CA-C-O     | 5.76  | 126.59      | 119.97   |
| 1   | A1    | 241 | ILE  | CA-CB-CG1  | -5.75 | 100.62      | 110.40   |
| 5   | Q1    | 184 | SER  | CA-C-O     | -5.75 | 114.50      | 121.05   |
| 7   | G1    | 58  | VAL  | N-CA-CB    | 5.75  | 117.65      | 110.47   |
| 4   | D1    | 201 | ARG  | CA-CB-CG   | 5.75  | 125.59      | 114.10   |
| 2   | B1    | 310 | SER  | N-CA-C     | 5.74  | 118.81      | 109.06   |
| 2   | B1    | 157 | ALA  | N-CA-C     | 5.73  | 117.20      | 111.07   |
| 1   | M1    | 339 | GLN  | O-C-N      | 5.73  | 130.21      | 122.59   |
| 1   | M1    | 138 | LEU  | O-C-N      | 5.72  | 129.13      | 122.20   |
| 57  | B3    | 190 | GLY  | N-CA-C     | 5.72  | 117.71      | 110.38   |
| 1   | A1    | 434 | TYR  | CB-CG-CD1  | 5.72  | 129.38      | 120.80   |
| 5   | Q1    | 32  | ARG  | CB-CA-C    | 5.72  | 120.41      | 110.68   |
| 1   | M1    | 56  | GLY  | O-C-N      | -5.72 | 115.26      | 122.70   |
| 3   | O1    | 63  | PHE  | O-C-N      | 5.72  | 129.12      | 122.20   |
| 1   | M1    | 436 | ARG  | CA-C-N     | -5.71 | 112.08      | 121.34   |
| 1   | M1    | 436 | ARG  | C-N-CA     | -5.71 | 112.08      | 121.34   |
| 35  | R2    | 62  | THR  | N-CA-C     | -5.71 | 107.31      | 114.56   |
| 65  | J3    | 25  | GLY  | N-CA-C     | 5.71  | 118.94      | 110.60   |
| 6   | R1    | 22  | ASN  | N-CA-C     | -5.71 | 106.15      | 113.23   |
| 3   | C1    | 153 | ILE  | CA-C-N     | 5.71  | 126.97      | 119.84   |
| 3   | C1    | 153 | ILE  | C-N-CA     | 5.71  | 126.97      | 119.84   |
| 3   | O1    | 185 | LEU  | CA-C-O     | -5.71 | 113.31      | 118.79   |
| 4   | P1    | 50  | HIS  | N-CA-C     | -5.71 | 106.16      | 113.23   |
| 3   | C1    | 15  | ASN  | OD1-CG-ND2 | 5.70  | 128.30      | 122.60   |
| 2   | B1    | 139 | ALA  | CA-C-O     | 5.70  | 126.81      | 120.82   |
| 1   | M1    | 93  | GLU  | CA-CB-CG   | -5.70 | 102.70      | 114.10   |
| 3   | O1    | 46  | LEU  | N-CA-C     | -5.70 | 104.98      | 111.14   |
| 6   | F1    | 24  | ALA  | CA-C-O     | 5.70  | 126.95      | 120.80   |
| 3   | O1    | 256 | TYR  | CA-C-O     | -5.70 | 112.80      | 120.15   |
| 1   | A1    | 23  | LEU  | CA-C-N     | -5.70 | 114.86      | 122.72   |
| 1   | A1    | 23  | LEU  | C-N-CA     | -5.70 | 114.86      | 122.72   |
| 3   | C1    | 97  | HIS  | CB-CG-ND1  | 5.70  | 131.24      | 122.70   |
| 4   | D1    | 203 | ARG  | CA-C-O     | 5.70  | 127.33      | 121.07   |
| 3   | O1    | 22  | PRO  | N-CA-CB    | 5.70  | 108.24      | 103.17   |
| 46  | c2    | 36  | PRO  | CA-C-N     | 5.70  | 140.67      | 127.00   |
| 46  | c2    | 36  | PRO  | C-N-CA     | 5.70  | 140.67      | 127.00   |
| 1   | A1    | 193 | PRO  | N-CA-CB    | 5.69  | 108.86      | 102.60   |
| 1   | A1    | 392 | LEU  | N-CA-C     | 5.69  | 117.94      | 111.11   |
| 2   | N1    | 108 | THR  | N-CA-C     | 5.69  | 118.08      | 110.35   |
| 4   | D1    | 9   | SER  | N-CA-C     | -5.69 | 101.09      | 109.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | A3    | 129 | TYR  | CB-CA-C     | -5.68 | 100.50      | 109.42   |
| 1   | A1    | 368 | HIS  | CA-CB-CG    | -5.68 | 108.12      | 113.80   |
| 6   | R1    | 23  | ALA  | N-CA-C      | -5.68 | 104.78      | 110.97   |
| 9   | U1    | 51  | CYS  | CA-C-N      | 5.68  | 128.46      | 120.28   |
| 9   | U1    | 51  | CYS  | C-N-CA      | 5.68  | 128.46      | 120.28   |
| 4   | P1    | 195 | GLU  | CA-C-N      | 5.68  | 125.53      | 119.28   |
| 4   | P1    | 195 | GLU  | C-N-CA      | 5.68  | 125.53      | 119.28   |
| 2   | N1    | 254 | HIS  | CA-CB-CG    | 5.68  | 119.48      | 113.80   |
| 1   | A1    | 418 | GLN  | OE1-CD-NE2  | 5.68  | 128.28      | 122.60   |
| 1   | M1    | 47  | TYR  | N-CA-C      | -5.68 | 106.52      | 113.50   |
| 2   | B1    | 102 | ARG  | CD-NE-CZ    | -5.67 | 116.46      | 124.40   |
| 3   | C1    | 77  | TRP  | CD2-CE3-CZ3 | -5.67 | 111.22      | 118.60   |
| 59  | D3    | 129 | ALA  | CA-C-N      | 5.67  | 126.93      | 119.84   |
| 59  | D3    | 129 | ALA  | C-N-CA      | 5.67  | 126.93      | 119.84   |
| 2   | B1    | 65  | THR  | OG1-CB-CG2  | 5.67  | 120.64      | 109.30   |
| 2   | N1    | 187 | THR  | CA-C-N      | 5.67  | 126.92      | 119.84   |
| 2   | N1    | 187 | THR  | C-N-CA      | 5.67  | 126.92      | 119.84   |
| 1   | M1    | 32  | GLN  | CA-C-N      | 5.66  | 126.92      | 119.84   |
| 1   | M1    | 32  | GLN  | C-N-CA      | 5.66  | 126.92      | 119.84   |
| 2   | B1    | 61  | ASN  | OD1-CG-ND2  | -5.66 | 116.94      | 122.60   |
| 3   | O1    | 100 | ARG  | N-CA-C      | -5.65 | 105.11      | 112.23   |
| 3   | C1    | 22  | PRO  | N-CA-CB     | 5.65  | 109.18      | 103.25   |
| 6   | F1    | 43  | VAL  | O-C-N       | -5.65 | 115.51      | 122.57   |
| 1   | A1    | 242 | CYS  | N-CA-C      | 5.65  | 118.45      | 109.24   |
| 3   | C1    | 16  | ASN  | OD1-CG-ND2  | -5.64 | 116.96      | 122.60   |
| 3   | C1    | 96  | MET  | N-CA-C      | -5.64 | 105.21      | 111.36   |
| 3   | C1    | 191 | ALA  | N-CA-C      | -5.64 | 105.04      | 111.07   |
| 3   | O1    | 264 | THR  | CB-CA-C     | -5.64 | 102.32      | 109.65   |
| 1   | A1    | 11  | VAL  | N-CA-C      | 5.64  | 114.26      | 109.02   |
| 1   | A1    | 279 | HIS  | O-C-N       | -5.63 | 117.17      | 123.48   |
| 3   | O1    | 257 | THR  | CB-CA-C     | -5.63 | 103.43      | 109.85   |
| 9   | U1    | 56  | ARG  | CA-C-N      | 5.63  | 128.71      | 121.27   |
| 9   | U1    | 56  | ARG  | C-N-CA      | 5.63  | 128.71      | 121.27   |
| 1   | M1    | 428 | ILE  | O-C-N       | -5.63 | 116.30      | 122.05   |
| 2   | N1    | 201 | SER  | N-CA-C      | 5.63  | 117.11      | 110.97   |
| 4   | P1    | 30  | PHE  | CA-CB-CG    | -5.63 | 108.17      | 113.80   |
| 1   | M1    | 154 | HIS  | CA-CB-CG    | 5.63  | 119.43      | 113.80   |
| 4   | P1    | 38  | SER  | CA-C-N      | 5.62  | 128.38      | 120.28   |
| 4   | P1    | 38  | SER  | C-N-CA      | 5.62  | 128.38      | 120.28   |
| 2   | N1    | 165 | ALA  | CA-C-O      | 5.62  | 126.28      | 119.31   |
| 1   | A1    | 205 | HIS  | CA-CB-CG    | -5.62 | 108.19      | 113.80   |
| 1   | M1    | 292 | SER  | CA-C-O      | 5.61  | 124.07      | 119.36   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5   | Q1    | 76  | ILE  | CA-C-O    | -5.61 | 115.41      | 121.19   |
| 8   | H1    | 63  | HIS  | CA-CB-CG  | -5.61 | 108.19      | 113.80   |
| 57  | B3    | 104 | TRP  | N-CA-C    | 5.61  | 122.74      | 110.80   |
| 2   | N1    | 45  | SER  | O-C-N     | -5.60 | 116.63      | 123.19   |
| 3   | O1    | 56  | THR  | O-C-N     | -5.60 | 116.35      | 123.24   |
| 1   | A1    | 414 | TYR  | N-CA-C    | 5.59  | 120.23      | 112.90   |
| 1   | M1    | 376 | CYS  | CA-CB-SG  | -5.59 | 101.53      | 114.40   |
| 4   | P1    | 109 | LEU  | CA-C-N    | 5.59  | 126.14      | 120.38   |
| 4   | P1    | 109 | LEU  | C-N-CA    | 5.59  | 126.14      | 120.38   |
| 2   | B1    | 403 | ASP  | CA-CB-CG  | -5.58 | 107.02      | 112.60   |
| 3   | O1    | 45  | ILE  | CB-CA-C   | -5.58 | 104.83      | 111.81   |
| 8   | H1    | 54  | CYS  | CA-C-N    | 5.58  | 127.70      | 120.44   |
| 8   | H1    | 54  | CYS  | C-N-CA    | 5.58  | 127.70      | 120.44   |
| 3   | C1    | 111 | GLU  | CA-C-O    | -5.58 | 114.93      | 120.90   |
| 3   | O1    | 35  | SER  | CA-C-N    | 5.57  | 128.01      | 120.38   |
| 3   | O1    | 35  | SER  | C-N-CA    | 5.57  | 128.01      | 120.38   |
| 3   | O1    | 196 | HIS  | N-CA-C    | -5.57 | 105.11      | 111.07   |
| 2   | B1    | 197 | ASN  | N-CA-C    | 5.57  | 117.43      | 111.36   |
| 3   | O1    | 126 | THR  | CA-C-O    | -5.56 | 114.98      | 120.82   |
| 6   | R1    | 99  | ARG  | CA-C-N    | -5.56 | 112.83      | 120.28   |
| 6   | R1    | 99  | ARG  | C-N-CA    | -5.56 | 112.83      | 120.28   |
| 3   | C1    | 143 | ALA  | CA-C-N    | -5.56 | 113.21      | 120.44   |
| 3   | C1    | 143 | ALA  | C-N-CA    | -5.56 | 113.21      | 120.44   |
| 3   | O1    | 199 | PHE  | CB-CG-CD2 | 5.56  | 130.15      | 120.70   |
| 8   | T1    | 63  | HIS  | CA-CB-CG  | -5.56 | 108.24      | 113.80   |
| 3   | C1    | 120 | LEU  | CA-C-O    | 5.56  | 126.85      | 120.90   |
| 1   | A1    | 22  | GLY  | N-CA-C    | -5.55 | 107.12      | 114.95   |
| 4   | P1    | 16  | GLY  | N-CA-C    | 5.55  | 120.15      | 112.37   |
| 7   | S1    | 19  | SER  | CA-C-N    | 5.55  | 125.02      | 119.24   |
| 7   | S1    | 19  | SER  | C-N-CA    | 5.55  | 125.02      | 119.24   |
| 1   | A1    | 360 | LEU  | N-CA-C    | -5.55 | 105.31      | 111.36   |
| 4   | D1    | 31  | GLN  | CA-C-O    | -5.55 | 114.96      | 120.90   |
| 3   | C1    | 21  | LEU  | N-CA-C    | 5.55  | 116.69      | 109.64   |
| 1   | A1    | 69  | ASN  | CA-C-O    | 5.55  | 126.83      | 121.00   |
| 3   | C1    | 269 | LYS  | CA-C-N    | 5.55  | 125.86      | 119.92   |
| 3   | C1    | 269 | LYS  | C-N-CA    | 5.55  | 125.86      | 119.92   |
| 1   | M1    | 415 | PHE  | CA-CB-CG  | 5.55  | 119.35      | 113.80   |
| 13  | 32    | 20  | ILE  | N-CA-C    | -5.55 | 106.42      | 112.80   |
| 62  | G3    | 72  | ASN  | CA-C-N    | 5.55  | 125.91      | 119.47   |
| 62  | G3    | 72  | ASN  | C-N-CA    | 5.55  | 125.91      | 119.47   |
| 64  | I3    | 20  | HIS  | N-CA-C    | 5.55  | 118.09      | 111.71   |
| 1   | M1    | 300 | THR  | CA-CB-OG1 | 5.54  | 117.92      | 109.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | O1    | 185 | LEU  | O-C-N       | 5.54  | 124.76      | 120.38   |
| 3   | C1    | 182 | HIS  | N-CA-C      | -5.54 | 105.24      | 111.28   |
| 51  | j2    | 22  | PRO  | C-N-CD      | -5.54 | 108.41      | 120.60   |
| 61  | F3    | 82  | CYS  | CA-C-N      | 5.54  | 125.37      | 119.28   |
| 61  | F3    | 82  | CYS  | C-N-CA      | 5.54  | 125.37      | 119.28   |
| 2   | B1    | 320 | GLY  | CA-C-O      | 5.54  | 126.51      | 121.47   |
| 3   | C1    | 123 | VAL  | CA-C-N      | -5.54 | 111.26      | 120.68   |
| 3   | C1    | 123 | VAL  | C-N-CA      | -5.54 | 111.26      | 120.68   |
| 4   | D1    | 206 | LEU  | N-CA-CB     | 5.54  | 119.13      | 109.72   |
| 5   | Q1    | 47  | VAL  | N-CA-C      | 5.54  | 116.93      | 110.62   |
| 58  | C3    | 188 | ILE  | CB-CA-C     | -5.54 | 104.67      | 112.14   |
| 1   | M1    | 341 | GLN  | CA-C-O      | -5.53 | 114.56      | 120.42   |
| 5   | Q1    | 91  | TRP  | CB-CG-CD2   | 5.53  | 134.55      | 126.80   |
| 1   | M1    | 217 | SER  | N-CA-CB     | -5.53 | 102.52      | 110.87   |
| 7   | S1    | 12  | HIS  | CA-CB-CG    | -5.53 | 108.27      | 113.80   |
| 4   | D1    | 114 | SER  | CA-CB-OG    | 5.53  | 122.16      | 111.10   |
| 1   | M1    | 189 | HIS  | CA-CB-CG    | 5.53  | 119.33      | 113.80   |
| 5   | Q1    | 40  | THR  | CA-CB-CG2   | 5.53  | 119.89      | 110.50   |
| 3   | C1    | 164 | ILE  | CA-C-O      | -5.52 | 115.53      | 121.27   |
| 3   | C1    | 205 | SER  | N-CA-C      | 5.52  | 118.18      | 109.96   |
| 1   | A1    | 395 | TRP  | CD2-CE2-CZ2 | 5.51  | 127.92      | 122.40   |
| 5   | Q1    | 29  | SER  | CA-C-N      | 5.51  | 127.67      | 120.28   |
| 5   | Q1    | 29  | SER  | C-N-CA      | 5.51  | 127.67      | 120.28   |
| 3   | O1    | 282 | ARG  | CD-NE-CZ    | -5.51 | 116.68      | 124.40   |
| 67  | L3    | 16  | GLU  | N-CA-C      | 5.51  | 117.37      | 111.36   |
| 4   | D1    | 40  | CYS  | CB-CA-C     | 5.51  | 116.27      | 109.16   |
| 24  | F2    | 97  | MET  | CA-C-N      | 5.51  | 140.22      | 127.00   |
| 24  | F2    | 97  | MET  | C-N-CA      | 5.51  | 140.22      | 127.00   |
| 3   | C1    | 18  | PHE  | CA-C-N      | 5.50  | 128.61      | 120.74   |
| 3   | C1    | 18  | PHE  | C-N-CA      | 5.50  | 128.61      | 120.74   |
| 2   | B1    | 190 | GLU  | CA-C-O      | -5.50 | 115.02      | 120.90   |
| 65  | J3    | 2   | GLU  | N-CA-C      | 5.50  | 122.51      | 110.80   |
| 1   | A1    | 46  | ARG  | NE-CZ-NH2   | -5.49 | 114.25      | 119.20   |
| 7   | G1    | 15  | THR  | N-CA-C      | 5.49  | 118.43      | 109.59   |
| 10  | V1    | 8   | ARG  | CA-C-N      | 5.49  | 127.95      | 120.54   |
| 10  | V1    | 8   | ARG  | C-N-CA      | 5.49  | 127.95      | 120.54   |
| 3   | C1    | 188 | ILE  | N-CA-CB     | 5.48  | 117.59      | 110.57   |
| 43  | Z2    | 41  | LEU  | CA-C-N      | 5.48  | 131.57      | 121.70   |
| 43  | Z2    | 41  | LEU  | C-N-CA      | 5.48  | 131.57      | 121.70   |
| 1   | M1    | 252 | HIS  | CA-CB-CG    | -5.48 | 108.32      | 113.80   |
| 1   | A1    | 208 | LEU  | N-CA-C      | -5.48 | 105.00      | 110.97   |
| 6   | R1    | 98  | ILE  | O-C-N       | -5.48 | 116.46      | 121.94   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N1    | 329 | GLN  | CB-CA-C   | 5.47  | 119.92      | 110.45   |
| 4   | D1    | 208 | MET  | CA-CB-CG  | 5.47  | 125.04      | 114.10   |
| 1   | M1    | 375 | VAL  | O-C-N     | 5.47  | 127.25      | 121.89   |
| 9   | U1    | 58  | GLN  | N-CA-C    | 5.47  | 118.40      | 109.59   |
| 5   | Q1    | 69  | LEU  | CA-C-N    | 5.47  | 128.06      | 120.29   |
| 5   | Q1    | 69  | LEU  | C-N-CA    | 5.47  | 128.06      | 120.29   |
| 4   | D1    | 182 | VAL  | CA-CB-CG1 | 5.46  | 119.69      | 110.40   |
| 5   | E1    | 49  | TYR  | N-CA-C    | -5.46 | 104.36      | 111.02   |
| 1   | A1    | 149 | VAL  | N-CA-CB   | 5.46  | 116.94      | 110.55   |
| 2   | B1    | 85  | ILE  | N-CA-C    | 5.46  | 116.09      | 110.36   |
| 3   | C1    | 26  | ASN  | O-C-N     | -5.46 | 116.57      | 123.12   |
| 2   | B1    | 46  | ARG  | CB-CA-C   | -5.46 | 102.65      | 110.62   |
| 2   | B1    | 44  | ALA  | N-CA-C    | 5.46  | 117.41      | 108.52   |
| 6   | R1    | 32  | MET  | N-CA-CB   | -5.45 | 102.06      | 111.55   |
| 55  | e2    | 82  | SER  | N-CA-C    | 5.45  | 122.42      | 110.80   |
| 4   | D1    | 213 | GLY  | CA-C-O    | 5.45  | 125.88      | 119.45   |
| 56  | A3    | 245 | ILE  | N-CA-C    | -5.45 | 104.24      | 111.05   |
| 19  | A2    | 507 | THR  | CA-C-N    | 5.45  | 131.50      | 121.70   |
| 19  | A2    | 507 | THR  | C-N-CA    | 5.45  | 131.50      | 121.70   |
| 46  | c2    | 36  | PRO  | C-N-CD    | -5.45 | 108.62      | 120.60   |
| 4   | D1    | 109 | LEU  | CA-C-N    | 5.44  | 125.99      | 120.38   |
| 4   | D1    | 109 | LEU  | C-N-CA    | 5.44  | 125.99      | 120.38   |
| 4   | D1    | 191 | ARG  | CA-C-O    | -5.44 | 114.66      | 121.02   |
| 7   | G1    | 10  | VAL  | CA-C-O    | 5.44  | 125.64      | 120.25   |
| 3   | O1    | 261 | PRO  | N-CA-CB   | 5.44  | 108.96      | 103.25   |
| 6   | R1    | 16  | ILE  | N-CA-C    | -5.44 | 105.55      | 110.82   |
| 7   | S1    | 12  | HIS  | CA-C-N    | -5.44 | 115.87      | 123.10   |
| 7   | S1    | 12  | HIS  | C-N-CA    | -5.44 | 115.87      | 123.10   |
| 2   | B1    | 309 | VAL  | N-CA-C    | 5.43  | 115.02      | 108.06   |
| 3   | C1    | 195 | VAL  | CA-C-N    | 5.43  | 127.82      | 120.65   |
| 3   | C1    | 195 | VAL  | C-N-CA    | 5.43  | 127.82      | 120.65   |
| 4   | P1    | 48  | TYR  | CA-C-N    | 5.43  | 130.17      | 122.24   |
| 4   | P1    | 48  | TYR  | C-N-CA    | 5.43  | 130.17      | 122.24   |
| 1   | A1    | 373 | THR  | O-C-N     | -5.42 | 115.47      | 120.51   |
| 1   | A1    | 443 | TRP  | N-CA-C    | 5.42  | 119.20      | 107.49   |
| 5   | E1    | 71  | MET  | CA-C-O    | -5.42 | 114.68      | 120.42   |
| 1   | M1    | 421 | ALA  | CB-CA-C   | 5.42  | 119.62      | 110.79   |
| 1   | A1    | 142 | ASP  | CA-C-O    | 5.42  | 126.05      | 119.49   |
| 9   | I1    | 51  | CYS  | N-CA-C    | 5.42  | 118.44      | 109.94   |
| 3   | O1    | 32  | ASN  | CA-CB-CG  | -5.42 | 107.19      | 112.60   |
| 6   | F1    | 76  | PRO  | N-CA-CB   | 5.41  | 108.06      | 103.35   |
| 5   | Q1    | 10  | PHE  | CA-CB-CG  | -5.41 | 108.39      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F1    | 97  | VAL  | N-CA-CB     | -5.41 | 102.31      | 111.23   |
| 7   | G1    | 18  | LEU  | O-C-N       | -5.41 | 115.53      | 122.94   |
| 3   | C1    | 74  | ASN  | N-CA-C      | 5.41  | 116.93      | 109.15   |
| 12  | 22    | 40  | ILE  | CA-C-N      | 5.41  | 125.62      | 120.43   |
| 12  | 22    | 40  | ILE  | C-N-CA      | 5.41  | 125.62      | 120.43   |
| 3   | C1    | 19  | ILE  | N-CA-C      | 5.40  | 116.06      | 110.82   |
| 1   | A1    | 395 | TRP  | NE1-CE2-CZ2 | -5.40 | 122.00      | 130.10   |
| 34  | Q2    | 141 | PRO  | CA-C-N      | 5.39  | 128.90      | 120.82   |
| 34  | Q2    | 141 | PRO  | C-N-CA      | 5.39  | 128.90      | 120.82   |
| 1   | M1    | 435 | ASN  | CB-CG-OD1   | -5.39 | 110.03      | 120.80   |
| 3   | O1    | 201 | HIS  | CA-CB-CG    | -5.39 | 108.41      | 113.80   |
| 5   | E1    | 75  | GLU  | CA-C-O      | -5.38 | 111.65      | 120.80   |
| 1   | M1    | 390 | ILE  | N-CA-CB     | 5.38  | 118.75      | 111.21   |
| 3   | O1    | 234 | LEU  | N-CA-C      | -5.38 | 105.49      | 111.36   |
| 1   | A1    | 161 | THR  | CA-C-N      | 5.38  | 125.20      | 119.28   |
| 1   | A1    | 161 | THR  | C-N-CA      | 5.38  | 125.20      | 119.28   |
| 6   | F1    | 90  | LEU  | O-C-N       | 5.38  | 129.54      | 122.33   |
| 7   | G1    | 19  | SER  | CA-C-N      | 5.38  | 125.45      | 119.32   |
| 7   | G1    | 19  | SER  | C-N-CA      | 5.38  | 125.45      | 119.32   |
| 3   | C1    | 239 | LEU  | CD1-CG-CD2  | -5.38 | 98.97       | 110.80   |
| 2   | N1    | 92  | VAL  | N-CA-CB     | -5.38 | 105.32      | 112.26   |
| 6   | R1    | 36  | THR  | CA-C-O      | 5.38  | 126.17      | 119.12   |
| 1   | A1    | 94  | HIS  | CB-CA-C     | -5.37 | 104.06      | 110.94   |
| 1   | M1    | 419 | CYS  | CA-CB-SG    | 5.37  | 126.76      | 114.40   |
| 1   | M1    | 315 | ALA  | CA-C-O      | 5.37  | 126.46      | 120.82   |
| 1   | A1    | 343 | MET  | O-C-N       | -5.37 | 115.45      | 122.59   |
| 2   | B1    | 89  | ILE  | O-C-N       | -5.37 | 116.66      | 121.87   |
| 1   | A1    | 428 | ILE  | CA-CB-CG1   | 5.37  | 119.52      | 110.40   |
| 1   | M1    | 415 | PHE  | CA-C-O      | 5.36  | 126.27      | 119.78   |
| 56  | A3    | 305 | PHE  | N-CA-C      | 5.36  | 118.92      | 112.38   |
| 4   | P1    | 84  | PRO  | N-CA-CB     | 5.36  | 107.82      | 103.32   |
| 10  | V1    | 19  | THR  | CA-CB-OG1   | -5.36 | 101.56      | 109.60   |
| 56  | A3    | 159 | LEU  | N-CA-C      | -5.36 | 105.52      | 111.36   |
| 4   | D1    | 191 | ARG  | CA-C-N      | 5.35  | 127.71      | 120.38   |
| 4   | D1    | 191 | ARG  | C-N-CA      | 5.35  | 127.71      | 120.38   |
| 4   | D1    | 32  | VAL  | CB-CA-C     | -5.35 | 105.03      | 111.88   |
| 7   | G1    | 50  | PRO  | N-CA-CB     | 5.35  | 108.27      | 103.08   |
| 3   | O1    | 141 | TRP  | CA-C-N      | 5.35  | 125.88      | 119.94   |
| 3   | O1    | 141 | TRP  | C-N-CA      | 5.35  | 125.88      | 119.94   |
| 2   | B1    | 107 | TYR  | CA-C-N      | 5.35  | 128.83      | 120.75   |
| 2   | B1    | 107 | TYR  | C-N-CA      | 5.35  | 128.83      | 120.75   |
| 10  | J1    | 55  | ILE  | N-CA-C      | 5.35  | 118.95      | 112.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A1    | 170 | PRO  | N-CA-CB     | 5.34  | 108.86      | 103.25   |
| 2   | N1    | 394 | PRO  | CA-C-N      | 5.34  | 126.52      | 119.84   |
| 2   | N1    | 394 | PRO  | C-N-CA      | 5.34  | 126.52      | 119.84   |
| 3   | C1    | 210 | GLY  | CA-C-N      | 5.34  | 132.09      | 122.43   |
| 3   | C1    | 210 | GLY  | C-N-CA      | 5.34  | 132.09      | 122.43   |
| 9   | U1    | 78  | TYR  | CA-CB-CG    | 5.34  | 123.50      | 113.90   |
| 3   | C1    | 175 | LEU  | CA-C-O      | 5.33  | 126.08      | 119.79   |
| 3   | O1    | 259 | ALA  | CA-C-O      | -5.33 | 114.68      | 120.81   |
| 3   | C1    | 15  | ASN  | CA-CB-CG    | -5.32 | 107.28      | 112.60   |
| 3   | C1    | 361 | LEU  | CA-C-O      | -5.32 | 114.89      | 120.63   |
| 4   | P1    | 209 | LEU  | O-C-N       | -5.32 | 115.74      | 122.17   |
| 1   | A1    | 436 | ARG  | CD-NE-CZ    | -5.31 | 116.96      | 124.40   |
| 5   | Q1    | 65  | SER  | O-C-N       | -5.31 | 116.59      | 122.86   |
| 3   | O1    | 115 | ILE  | CA-CB-CG1   | 5.31  | 119.43      | 110.40   |
| 5   | Q1    | 172 | ARG  | CA-C-N      | 5.31  | 129.78      | 121.76   |
| 5   | Q1    | 172 | ARG  | C-N-CA      | 5.31  | 129.78      | 121.76   |
| 2   | B1    | 60  | SER  | CA-CB-OG    | -5.31 | 100.49      | 111.10   |
| 4   | D1    | 201 | ARG  | CD-NE-CZ    | -5.31 | 116.97      | 124.40   |
| 3   | O1    | 199 | PHE  | CD1-CG-CD2  | -5.31 | 110.64      | 118.60   |
| 2   | B1    | 75  | LEU  | O-C-N       | 5.30  | 129.17      | 122.65   |
| 32  | O2    | 42  | GLU  | CA-C-N      | 5.30  | 124.57      | 120.33   |
| 32  | O2    | 42  | GLU  | C-N-CA      | 5.30  | 124.57      | 120.33   |
| 56  | A3    | 372 | TYR  | N-CA-C      | -5.30 | 105.40      | 111.07   |
| 1   | M1    | 145 | MET  | CA-C-N      | -5.30 | 113.12      | 120.38   |
| 1   | M1    | 145 | MET  | C-N-CA      | -5.30 | 113.12      | 120.38   |
| 1   | A1    | 342 | TRP  | CD2-CE2-CZ2 | 5.30  | 127.70      | 122.40   |
| 2   | B1    | 33  | LEU  | O-C-N       | 5.29  | 129.30      | 123.16   |
| 1   | M1    | 440 | GLY  | N-CA-C      | -5.29 | 107.75      | 114.16   |
| 1   | A1    | 153 | LEU  | O-C-N       | 5.29  | 127.74      | 122.08   |
| 3   | C1    | 126 | THR  | N-CA-CB     | 5.29  | 118.40      | 109.78   |
| 2   | N1    | 274 | VAL  | O-C-N       | 5.29  | 127.28      | 121.83   |
| 3   | O1    | 106 | SER  | CA-C-O      | 5.29  | 125.88      | 119.38   |
| 1   | M1    | 260 | PRO  | N-CA-CB     | 5.29  | 108.36      | 103.39   |
| 4   | D1    | 239 | PRO  | CA-C-N      | 5.28  | 126.44      | 119.84   |
| 4   | D1    | 239 | PRO  | C-N-CA      | 5.28  | 126.44      | 119.84   |
| 2   | B1    | 133 | ARG  | NE-CZ-NH1   | 5.28  | 126.78      | 121.50   |
| 2   | N1    | 162 | ASN  | CB-CA-C     | 5.28  | 119.51      | 110.74   |
| 1   | M1    | 392 | LEU  | N-CA-CB     | 5.28  | 117.81      | 109.94   |
| 3   | O1    | 45  | ILE  | O-C-N       | 5.28  | 127.38      | 121.94   |
| 3   | C1    | 135 | TRP  | O-C-N       | 5.28  | 128.91      | 122.58   |
| 1   | A1    | 358 | LYS  | CA-C-N      | 5.27  | 127.61      | 120.38   |
| 1   | A1    | 358 | LYS  | C-N-CA      | 5.27  | 127.61      | 120.38   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A1    | 247 | GLY  | O-C-N     | -5.27 | 117.08      | 122.19   |
| 5   | Q1    | 91  | TRP  | CB-CG-CD1 | -5.27 | 118.99      | 126.90   |
| 1   | M1    | 25  | VAL  | CA-C-N    | -5.27 | 114.32      | 122.59   |
| 1   | M1    | 25  | VAL  | C-N-CA    | -5.27 | 114.32      | 122.59   |
| 2   | N1    | 70  | ARG  | NE-CZ-NH2 | -5.27 | 114.46      | 119.20   |
| 3   | C1    | 260 | ASN  | CA-CB-CG  | 5.26  | 117.86      | 112.60   |
| 3   | O1    | 160 | LEU  | N-CA-C    | 5.26  | 117.43      | 111.11   |
| 1   | M1    | 428 | ILE  | CA-C-O    | 5.26  | 125.40      | 120.14   |
| 5   | Q1    | 136 | ILE  | N-CA-CB   | -5.26 | 106.22      | 111.90   |
| 5   | Q1    | 182 | VAL  | O-C-N     | 5.26  | 126.01      | 120.96   |
| 2   | B1    | 94  | GLY  | CA-C-N    | 5.26  | 131.41      | 122.37   |
| 2   | B1    | 94  | GLY  | C-N-CA    | 5.26  | 131.41      | 122.37   |
| 2   | N1    | 107 | TYR  | CA-C-N    | 5.25  | 128.68      | 120.75   |
| 2   | N1    | 107 | TYR  | C-N-CA    | 5.25  | 128.68      | 120.75   |
| 7   | S1    | 17  | SER  | CA-C-O    | -5.25 | 115.30      | 121.44   |
| 1   | A1    | 391 | PRO  | CA-C-N    | 5.25  | 127.63      | 120.54   |
| 1   | A1    | 391 | PRO  | C-N-CA    | 5.25  | 127.63      | 120.54   |
| 3   | O1    | 226 | ILE  | CA-C-O    | 5.25  | 126.42      | 120.85   |
| 4   | D1    | 46  | VAL  | N-CA-CB   | 5.25  | 116.98      | 111.00   |
| 3   | C1    | 356 | VAL  | O-C-N     | -5.25 | 116.78      | 121.87   |
| 6   | F1    | 99  | ARG  | O-C-N     | -5.25 | 116.08      | 122.11   |
| 4   | D1    | 46  | VAL  | CA-C-O    | 5.24  | 126.79      | 120.65   |
| 51  | j2    | 115 | GLU  | CA-C-N    | 5.24  | 131.14      | 121.70   |
| 51  | j2    | 115 | GLU  | C-N-CA    | 5.24  | 131.14      | 121.70   |
| 1   | M1    | 162 | PRO  | CB-CA-C   | -5.24 | 103.51      | 112.26   |
| 2   | N1    | 416 | LYS  | N-CA-C    | 5.24  | 117.74      | 111.71   |
| 5   | Q1    | 39  | VAL  | N-CA-C    | -5.24 | 105.60      | 110.53   |
| 6   | F1    | 55  | TYR  | CA-C-O    | -5.24 | 115.00      | 120.55   |
| 4   | P1    | 191 | ARG  | CD-NE-CZ  | -5.24 | 117.07      | 124.40   |
| 2   | B1    | 353 | SER  | CA-C-N    | 5.24  | 129.84      | 121.62   |
| 2   | B1    | 353 | SER  | C-N-CA    | 5.24  | 129.84      | 121.62   |
| 3   | O1    | 219 | PRO  | CA-C-O    | 5.24  | 126.83      | 121.23   |
| 36  | S2    | 199 | VAL  | N-CA-C    | -5.23 | 102.80      | 107.56   |
| 8   | H1    | 55  | THR  | CA-CB-OG1 | 5.23  | 117.44      | 109.60   |
| 58  | C3    | 99  | TRP  | N-CA-C    | -5.23 | 105.48      | 111.07   |
| 1   | A1    | 357 | GLY  | N-CA-C    | -5.22 | 106.08      | 112.77   |
| 3   | C1    | 355 | SER  | O-C-N     | -5.22 | 116.58      | 122.12   |
| 56  | A3    | 262 | SER  | N-CA-C    | -5.22 | 106.59      | 113.17   |
| 3   | O1    | 91  | PHE  | CA-CB-CG  | -5.22 | 108.58      | 113.80   |
| 4   | D1    | 41  | HIS  | CA-CB-CG  | 5.22  | 119.02      | 113.80   |
| 1   | M1    | 416 | TYR  | N-CA-CB   | 5.22  | 118.29      | 109.94   |
| 1   | A1    | 311 | ASN  | CA-C-N    | -5.21 | 115.85      | 122.37   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A1    | 311 | ASN  | C-N-CA     | -5.21 | 115.85      | 122.37   |
| 1   | A1    | 167 | VAL  | N-CA-C     | -5.21 | 105.31      | 110.62   |
| 3   | O1    | 39  | ILE  | CB-CG1-CD1 | 5.21  | 124.74      | 113.80   |
| 1   | M1    | 277 | ILE  | CB-CA-C    | -5.21 | 105.22      | 111.88   |
| 4   | P1    | 137 | PRO  | CA-C-N     | 5.21  | 126.01      | 120.13   |
| 4   | P1    | 137 | PRO  | C-N-CA     | 5.21  | 126.01      | 120.13   |
| 6   | F1    | 61  | ARG  | NE-CZ-NH1  | -5.21 | 116.30      | 121.50   |
| 2   | N1    | 138 | ALA  | N-CA-C     | 5.21  | 117.36      | 111.11   |
| 4   | P1    | 85  | GLY  | CA-C-N     | 5.21  | 128.61      | 120.75   |
| 4   | P1    | 85  | GLY  | C-N-CA     | 5.21  | 128.61      | 120.75   |
| 3   | C1    | 196 | HIS  | N-CA-CB    | 5.20  | 117.51      | 109.91   |
| 2   | N1    | 430 | LEU  | N-CA-C     | 5.20  | 119.30      | 111.81   |
| 56  | A3    | 353 | LEU  | N-CA-C     | -5.20 | 105.69      | 111.36   |
| 1   | A1    | 425 | PHE  | CA-C-N     | 5.20  | 130.03      | 121.87   |
| 1   | A1    | 425 | PHE  | C-N-CA     | 5.20  | 130.03      | 121.87   |
| 3   | C1    | 289 | GLY  | CA-C-O     | -5.20 | 114.78      | 120.40   |
| 56  | A3    | 6   | TRP  | N-CA-C     | 5.20  | 119.68      | 113.23   |
| 1   | A1    | 403 | ASP  | CA-C-N     | -5.20 | 112.41      | 120.31   |
| 1   | A1    | 403 | ASP  | C-N-CA     | -5.20 | 112.41      | 120.31   |
| 8   | H1    | 60  | ASP  | N-CA-C     | -5.20 | 106.62      | 113.12   |
| 3   | C1    | 233 | LEU  | CA-C-O     | -5.19 | 115.34      | 120.90   |
| 3   | C1    | 276 | PHE  | N-CA-CB    | 5.19  | 119.27      | 110.49   |
| 3   | O1    | 124 | MET  | N-CA-C     | 5.19  | 116.94      | 111.28   |
| 9   | I1    | 69  | SER  | CA-C-O     | -5.19 | 114.72      | 120.33   |
| 1   | M1    | 350 | THR  | CA-C-O     | -5.19 | 115.24      | 121.11   |
| 1   | A1    | 390 | ILE  | N-CA-CB    | 5.19  | 118.47      | 111.21   |
| 4   | D1    | 132 | THR  | CA-CB-OG1  | -5.19 | 101.82      | 109.60   |
| 2   | N1    | 57  | TYR  | CA-C-N     | -5.19 | 114.10      | 122.81   |
| 2   | N1    | 57  | TYR  | C-N-CA     | -5.19 | 114.10      | 122.81   |
| 55  | e2    | 67  | ASP  | N-CA-C     | -5.19 | 102.66      | 110.70   |
| 2   | N1    | 337 | ILE  | CA-C-O     | -5.19 | 115.67      | 121.17   |
| 4   | P1    | 175 | THR  | CA-C-O     | 5.19  | 124.10      | 119.59   |
| 63  | H3    | 22  | ASN  | N-CA-C     | 5.19  | 117.75      | 109.81   |
| 2   | B1    | 282 | GLY  | CA-C-N     | 5.18  | 126.32      | 119.84   |
| 2   | B1    | 282 | GLY  | C-N-CA     | 5.18  | 126.32      | 119.84   |
| 4   | P1    | 195 | GLU  | O-C-N      | -5.18 | 116.60      | 121.32   |
| 6   | F1    | 19  | TRP  | CA-C-N     | 5.18  | 127.54      | 120.54   |
| 6   | F1    | 19  | TRP  | C-N-CA     | 5.18  | 127.54      | 120.54   |
| 1   | A1    | 363 | ASN  | OD1-CG-ND2 | 5.18  | 127.78      | 122.60   |
| 2   | B1    | 83  | PHE  | CA-CB-CG   | -5.17 | 108.62      | 113.80   |
| 2   | B1    | 394 | PRO  | N-CA-CB    | 5.17  | 108.10      | 103.08   |
| 6   | F1    | 26  | PHE  | CA-CB-CG   | 5.17  | 118.97      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M1    | 329 | MET  | CA-C-N     | -5.17 | 114.41      | 122.37   |
| 1   | M1    | 329 | MET  | C-N-CA     | -5.17 | 114.41      | 122.37   |
| 3   | C1    | 230 | LEU  | CA-C-O     | -5.17 | 115.39      | 120.82   |
| 3   | C1    | 281 | LEU  | O-C-N      | -5.17 | 116.65      | 122.03   |
| 8   | T1    | 55  | THR  | CA-CB-OG1  | 5.17  | 117.36      | 109.60   |
| 2   | B1    | 173 | ALA  | O-C-N      | -5.17 | 114.74      | 122.39   |
| 2   | N1    | 246 | GLU  | N-CA-C     | 5.17  | 117.80      | 107.62   |
| 14  | 42    | 84  | LEU  | N-CA-C     | -5.16 | 108.74      | 114.62   |
| 56  | A3    | 401 | SER  | N-CA-C     | 5.16  | 119.71      | 113.41   |
| 3   | O1    | 79  | ILE  | N-CA-CB    | 5.16  | 116.24      | 110.51   |
| 61  | F3    | 38  | ALA  | N-CA-C     | 5.16  | 117.78      | 110.50   |
| 3   | O1    | 60  | THR  | CB-CA-C    | -5.16 | 102.56      | 110.81   |
| 8   | T1    | 55  | THR  | CA-C-O     | 5.15  | 126.01      | 120.70   |
| 4   | P1    | 195 | GLU  | CA-C-O     | 5.15  | 127.23      | 120.74   |
| 25  | G2    | 55  | VAL  | CA-C-N     | 5.15  | 131.38      | 121.54   |
| 25  | G2    | 55  | VAL  | C-N-CA     | 5.15  | 131.38      | 121.54   |
| 2   | N1    | 169 | ARG  | N-CA-C     | -5.15 | 106.13      | 112.72   |
| 10  | J1    | 54  | HIS  | CA-C-N     | 5.15  | 128.93      | 121.52   |
| 10  | J1    | 54  | HIS  | C-N-CA     | 5.15  | 128.93      | 121.52   |
| 4   | D1    | 38  | SER  | CA-C-N     | 5.15  | 127.69      | 120.28   |
| 4   | D1    | 38  | SER  | C-N-CA     | 5.15  | 127.69      | 120.28   |
| 58  | C3    | 107 | ALA  | CA-C-N     | 5.15  | 125.95      | 119.98   |
| 58  | C3    | 107 | ALA  | C-N-CA     | 5.15  | 125.95      | 119.98   |
| 3   | O1    | 35  | SER  | O-C-N      | -5.15 | 115.75      | 122.59   |
| 5   | E1    | 39  | VAL  | CB-CA-C    | -5.14 | 105.30      | 111.88   |
| 7   | S1    | 36  | ASN  | OD1-CG-ND2 | -5.14 | 117.46      | 122.60   |
| 2   | B1    | 429 | ASN  | CA-CB-CG   | -5.14 | 107.46      | 112.60   |
| 1   | M1    | 169 | GLY  | CA-C-N     | 5.14  | 125.14      | 119.90   |
| 1   | M1    | 169 | GLY  | C-N-CA     | 5.14  | 125.14      | 119.90   |
| 4   | P1    | 143 | LEU  | N-CA-C     | 5.14  | 116.55      | 107.61   |
| 65  | J3    | 9   | GLN  | N-CA-C     | -5.14 | 105.57      | 111.07   |
| 7   | S1    | 33  | GLY  | O-C-N      | 5.13  | 127.11      | 122.18   |
| 1   | A1    | 188 | ARG  | CA-C-N     | -5.13 | 113.70      | 122.11   |
| 1   | A1    | 188 | ARG  | C-N-CA     | -5.13 | 113.70      | 122.11   |
| 7   | G1    | 9   | ARG  | NE-CZ-NH1  | -5.13 | 116.37      | 121.50   |
| 4   | P1    | 195 | GLU  | CB-CG-CD   | 5.13  | 121.32      | 112.60   |
| 2   | B1    | 256 | ALA  | CA-C-O     | -5.13 | 115.31      | 121.11   |
| 1   | M1    | 319 | LEU  | CA-C-O     | 5.13  | 125.96      | 120.32   |
| 12  | 22    | 273 | ASN  | CA-C-N     | 5.13  | 131.34      | 121.54   |
| 12  | 22    | 273 | ASN  | C-N-CA     | 5.13  | 131.34      | 121.54   |
| 2   | N1    | 66  | SER  | N-CA-C     | -5.12 | 105.59      | 111.07   |
| 2   | N1    | 165 | ALA  | O-C-N      | -5.12 | 115.39      | 122.46   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 19  | A2    | 153 | PHE  | CA-C-N     | 5.12  | 130.91      | 121.70   |
| 19  | A2    | 153 | PHE  | C-N-CA     | 5.12  | 130.91      | 121.70   |
| 3   | C1    | 119 | LEU  | CA-C-O     | 5.12  | 126.70      | 121.07   |
| 7   | G1    | 12  | HIS  | N-CA-C     | 5.11  | 118.45      | 111.39   |
| 1   | M1    | 295 | ALA  | CA-C-O     | 5.11  | 125.97      | 120.70   |
| 5   | Q1    | 44  | THR  | OG1-CB-CG2 | 5.11  | 119.53      | 109.30   |
| 1   | A1    | 306 | SER  | O-C-N      | -5.11 | 115.79      | 122.59   |
| 4   | D1    | 122 | GLY  | O-C-N      | 5.11  | 128.31      | 122.33   |
| 56  | A3    | 377 | PHE  | N-CA-C     | 5.11  | 119.36      | 113.18   |
| 7   | G1    | 19  | SER  | CA-C-O     | -5.11 | 116.00      | 120.60   |
| 12  | 22    | 129 | ILE  | N-CA-C     | -5.10 | 106.94      | 113.22   |
| 1   | A1    | 436 | ARG  | NE-CZ-NH1  | -5.10 | 116.40      | 121.50   |
| 4   | P1    | 33  | TYR  | CA-C-O     | -5.10 | 115.46      | 121.07   |
| 11  | W1    | 36  | THR  | CA-C-O     | 5.10  | 129.47      | 120.80   |
| 2   | B1    | 314 | ALA  | CA-C-O     | -5.10 | 115.19      | 120.70   |
| 2   | N1    | 125 | ASN  | OD1-CG-ND2 | 5.10  | 127.70      | 122.60   |
| 2   | B1    | 21  | PRO  | N-CA-CB    | 5.10  | 108.61      | 103.00   |
| 1   | M1    | 100 | LYS  | N-CA-C     | -5.10 | 100.93      | 109.24   |
| 1   | M1    | 157 | ALA  | CA-C-O     | 5.10  | 125.25      | 119.18   |
| 3   | O1    | 26  | ASN  | CA-C-O     | -5.10 | 115.54      | 121.15   |
| 9   | I1    | 78  | TYR  | CA-CB-CG   | 5.10  | 123.08      | 113.90   |
| 4   | P1    | 206 | LEU  | CA-C-N     | -5.10 | 113.17      | 120.82   |
| 4   | P1    | 206 | LEU  | C-N-CA     | -5.10 | 113.17      | 120.82   |
| 5   | Q1    | 40  | THR  | O-C-N      | -5.10 | 116.79      | 122.09   |
| 1   | A1    | 326 | CYS  | N-CA-C     | 5.09  | 117.75      | 109.24   |
| 3   | O1    | 275 | LEU  | CA-C-O     | -5.09 | 115.06      | 121.02   |
| 7   | G1    | 15  | THR  | CA-C-O     | -5.09 | 115.31      | 120.71   |
| 4   | P1    | 153 | PHE  | CA-C-N     | 5.09  | 126.20      | 119.84   |
| 4   | P1    | 153 | PHE  | C-N-CA     | 5.09  | 126.20      | 119.84   |
| 36  | S2    | 305 | VAL  | N-CA-C     | -5.09 | 107.79      | 112.83   |
| 2   | B1    | 275 | LEU  | CB-CA-C    | -5.09 | 102.86      | 110.90   |
| 1   | M1    | 138 | LEU  | CA-C-N     | 5.08  | 127.34      | 120.38   |
| 1   | M1    | 138 | LEU  | C-N-CA     | 5.08  | 127.34      | 120.38   |
| 1   | M1    | 361 | LEU  | O-C-N      | 5.08  | 127.38      | 122.09   |
| 3   | O1    | 221 | HIS  | CA-C-O     | 5.08  | 123.81      | 119.13   |
| 21  | C2    | 124 | ARG  | CA-C-N     | 5.08  | 131.25      | 121.54   |
| 21  | C2    | 124 | ARG  | C-N-CA     | 5.08  | 131.25      | 121.54   |
| 2   | N1    | 59  | ASN  | OD1-CG-ND2 | -5.08 | 117.52      | 122.60   |
| 4   | P1    | 44  | ASP  | N-CA-C     | 5.08  | 116.90      | 111.36   |
| 8   | H1    | 47  | ARG  | CA-CB-CG   | 5.08  | 124.26      | 114.10   |
| 3   | C1    | 9   | PRO  | N-CA-CB    | 5.08  | 107.72      | 103.25   |
| 8   | H1    | 55  | THR  | CB-CA-C    | -5.08 | 102.91      | 110.88   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | M1    | 414 | TYR  | CA-C-O    | -5.08 | 113.80      | 119.79   |
| 6   | R1    | 34  | ASP  | CA-CB-CG  | -5.08 | 107.52      | 112.60   |
| 2   | B1    | 170 | ASN  | N-CA-C    | 5.07  | 119.08      | 112.13   |
| 3   | O1    | 197 | LEU  | N-CA-CB   | 5.07  | 117.58      | 110.12   |
| 3   | O1    | 373 | GLU  | CA-C-O    | 5.07  | 126.11      | 120.63   |
| 4   | P1    | 143 | LEU  | CB-CA-C   | -5.07 | 103.74      | 110.79   |
| 1   | A1    | 119 | ASN  | CA-CB-CG  | -5.07 | 107.53      | 112.60   |
| 2   | B1    | 266 | SER  | CA-C-O    | -5.07 | 115.53      | 121.46   |
| 64  | I3    | 2   | THR  | N-CA-C    | 5.07  | 116.12      | 108.46   |
| 2   | N1    | 172 | LEU  | N-CA-CB   | 5.07  | 119.26      | 110.39   |
| 56  | A3    | 70  | VAL  | N-CA-C    | 5.07  | 115.50      | 110.23   |
| 3   | C1    | 325 | PHE  | CB-CA-C   | -5.06 | 102.90      | 110.90   |
| 2   | N1    | 354 | ASN  | CA-C-N    | 5.06  | 125.09      | 119.32   |
| 2   | N1    | 354 | ASN  | C-N-CA    | 5.06  | 125.09      | 119.32   |
| 4   | D1    | 110 | PRO  | N-CA-CB   | 5.06  | 107.99      | 103.08   |
| 3   | O1    | 197 | LEU  | N-CA-C    | -5.06 | 105.76      | 111.28   |
| 35  | R2    | 154 | GLN  | CA-C-N    | 5.06  | 128.92      | 120.62   |
| 35  | R2    | 154 | GLN  | C-N-CA    | 5.06  | 128.92      | 120.62   |
| 57  | B3    | 66  | THR  | N-CA-C    | -5.06 | 107.76      | 114.04   |
| 56  | A3    | 378 | HIS  | CB-CG-CD2 | -5.06 | 124.62      | 131.20   |
| 1   | M1    | 11  | VAL  | CA-C-O    | 5.06  | 124.42      | 119.71   |
| 1   | M1    | 420 | PRO  | N-CA-C    | 5.06  | 119.16      | 111.11   |
| 32  | O2    | 76  | PRO  | CA-C-N    | 5.06  | 131.21      | 121.54   |
| 32  | O2    | 76  | PRO  | C-N-CA    | 5.06  | 131.21      | 121.54   |
| 4   | D1    | 30  | PHE  | CA-CB-CG  | -5.06 | 108.74      | 113.80   |
| 10  | J1    | 51  | LEU  | N-CA-C    | 5.06  | 118.06      | 109.76   |
| 2   | N1    | 21  | PRO  | N-CA-CB   | 5.06  | 108.56      | 103.00   |
| 7   | S1    | 5   | GLY  | CA-C-N    | 5.06  | 130.16      | 122.37   |
| 7   | S1    | 5   | GLY  | C-N-CA    | 5.06  | 130.16      | 122.37   |
| 57  | B3    | 165 | VAL  | CA-C-N    | 5.06  | 126.16      | 119.84   |
| 57  | B3    | 165 | VAL  | C-N-CA    | 5.06  | 126.16      | 119.84   |
| 5   | Q1    | 62  | MET  | CA-C-N    | 5.05  | 131.19      | 121.54   |
| 5   | Q1    | 62  | MET  | C-N-CA    | 5.05  | 131.19      | 121.54   |
| 3   | O1    | 358 | TYR  | N-CA-C    | 5.05  | 117.17      | 111.11   |
| 7   | G1    | 34  | ILE  | CA-C-N    | 5.05  | 124.65      | 119.05   |
| 7   | G1    | 34  | ILE  | C-N-CA    | 5.05  | 124.65      | 119.05   |
| 3   | C1    | 102 | LEU  | N-CA-C    | 5.04  | 117.67      | 111.82   |
| 3   | O1    | 227 | LYS  | CA-C-O    | -5.04 | 115.52      | 120.82   |
| 37  | T2    | 83  | LYS  | N-CA-C    | 5.04  | 120.96      | 109.81   |
| 14  | 42    | 370 | PRO  | N-CA-C    | 5.04  | 116.85      | 110.70   |
| 20  | B2    | 293 | LEU  | CA-C-N    | 5.04  | 131.16      | 121.54   |
| 20  | B2    | 293 | LEU  | C-N-CA    | 5.04  | 131.16      | 121.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | P1    | 111 | PRO  | N-CA-CB     | 5.04  | 107.79      | 103.31   |
| 1   | A1    | 89  | TYR  | CA-CB-CG    | 5.03  | 122.96      | 113.90   |
| 3   | C1    | 64  | SER  | N-CA-C      | -5.03 | 105.69      | 111.07   |
| 4   | P1    | 229 | VAL  | N-CA-C      | -5.03 | 105.08      | 110.36   |
| 1   | A1    | 163 | LEU  | CA-C-O      | 5.03  | 125.56      | 119.38   |
| 7   | S1    | 73  | ASN  | CA-C-N      | 5.03  | 126.03      | 120.45   |
| 7   | S1    | 73  | ASN  | C-N-CA      | 5.03  | 126.03      | 120.45   |
| 57  | B3    | 12  | ALA  | N-CA-C      | 5.03  | 117.45      | 109.96   |
| 3   | C1    | 143 | ALA  | O-C-N       | -5.03 | 116.42      | 122.15   |
| 3   | O1    | 185 | LEU  | CA-CB-CG    | 5.03  | 133.89      | 116.30   |
| 56  | A3    | 2   | PHE  | N-CA-C      | -5.03 | 105.69      | 111.07   |
| 3   | C1    | 361 | LEU  | O-C-N       | 5.02  | 127.44      | 122.12   |
| 3   | O1    | 216 | ASP  | CA-C-N      | -5.02 | 115.41      | 122.94   |
| 3   | O1    | 216 | ASP  | C-N-CA      | -5.02 | 115.41      | 122.94   |
| 4   | P1    | 150 | ASN  | CA-C-N      | 5.02  | 124.68      | 119.56   |
| 4   | P1    | 150 | ASN  | C-N-CA      | 5.02  | 124.68      | 119.56   |
| 30  | L2    | 39  | THR  | CA-C-N      | 5.02  | 131.13      | 121.54   |
| 30  | L2    | 39  | THR  | C-N-CA      | 5.02  | 131.13      | 121.54   |
| 4   | D1    | 150 | ASN  | CA-C-N      | 5.02  | 125.09      | 119.87   |
| 4   | D1    | 150 | ASN  | C-N-CA      | 5.02  | 125.09      | 119.87   |
| 4   | P1    | 92  | PRO  | N-CA-CB     | 5.02  | 107.32      | 103.30   |
| 1   | M1    | 23  | LEU  | CA-C-N      | -5.02 | 115.79      | 122.72   |
| 1   | M1    | 23  | LEU  | C-N-CA      | -5.02 | 115.79      | 122.72   |
| 1   | M1    | 101 | ALA  | N-CA-C      | 5.02  | 116.15      | 108.52   |
| 3   | O1    | 325 | PHE  | CG-CD2-CE2  | 5.02  | 129.23      | 120.70   |
| 6   | F1    | 47  | ILE  | CB-CG1-CD1  | 5.02  | 124.33      | 113.80   |
| 53  | 62    | 405 | ASN  | CA-C-N      | 5.02  | 131.12      | 121.54   |
| 53  | 62    | 405 | ASN  | C-N-CA      | 5.02  | 131.12      | 121.54   |
| 2   | B1    | 38  | LEU  | CB-CA-C     | -5.02 | 104.90      | 111.82   |
| 1   | M1    | 342 | TRP  | CD2-CE2-CZ2 | -5.02 | 117.38      | 122.40   |
| 3   | O1    | 190 | MET  | N-CA-CB     | 5.02  | 117.49      | 110.12   |
| 3   | O1    | 326 | TRP  | CA-C-O      | -5.01 | 115.22      | 120.63   |
| 56  | A3    | 378 | HIS  | N-CA-C      | -5.01 | 106.33      | 112.90   |
| 2   | B1    | 126 | VAL  | CB-CA-C     | -5.01 | 104.39      | 112.16   |
| 5   | Q1    | 89  | PHE  | CA-C-N      | -5.01 | 114.33      | 121.50   |
| 5   | Q1    | 89  | PHE  | C-N-CA      | -5.01 | 114.33      | 121.50   |
| 1   | A1    | 328 | HIS  | CA-C-O      | 5.01  | 125.54      | 119.38   |
| 3   | C1    | 329 | VAL  | CA-C-O      | -5.01 | 114.52      | 120.78   |
| 4   | P1    | 15  | ARG  | CA-C-N      | 5.01  | 125.66      | 120.60   |
| 4   | P1    | 15  | ARG  | C-N-CA      | 5.01  | 125.66      | 120.60   |
| 61  | F3    | 81  | ARG  | N-CA-C      | 5.01  | 117.61      | 109.24   |
| 4   | D1    | 84  | PRO  | N-CA-CB     | 5.01  | 107.53      | 103.32   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1   | M1    | 430 | GLN  | CG-CD-NE2 | 5.01 | 123.91      | 116.40   |
| 3   | O1    | 54  | HIS  | CA-C-N    | 5.00 | 132.13      | 122.07   |
| 3   | O1    | 54  | HIS  | C-N-CA    | 5.00 | 132.13      | 122.07   |

There are no chirality outliers.

All (133) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 52  | 12    | 199 | ASP  | Peptide   |
| 12  | 22    | 293 | TYR  | Peptide   |
| 12  | 22    | 45  | MET  | Peptide   |
| 14  | 42    | 224 | PRO  | Peptide   |
| 14  | 42    | 306 | PRO  | Peptide   |
| 14  | 42    | 369 | LEU  | Peptide   |
| 15  | 52    | 24  | SER  | Peptide   |
| 53  | 62    | 29  | PRO  | Peptide   |
| 53  | 62    | 352 | ASP  | Peptide   |
| 16  | 72    | 140 | ALA  | Peptide   |
| 16  | 72    | 170 | GLU  | Peptide   |
| 16  | 72    | 25  | SER  | Peptide   |
| 17  | 82    | 228 | PRO  | Peptide   |
| 18  | 92    | 150 | GLU  | Peptide   |
| 18  | 92    | 167 | LYS  | Peptide   |
| 18  | 92    | 75  | LYS  | Peptide   |
| 1   | A1    | 118 | GLN  | Mainchain |
| 1   | A1    | 122 | LEU  | Mainchain |
| 1   | A1    | 196 | VAL  | Mainchain |
| 1   | A1    | 210 | ASP  | Mainchain |
| 1   | A1    | 239 | SER  | Mainchain |
| 1   | A1    | 242 | CYS  | Mainchain |
| 1   | A1    | 244 | ARG  | Mainchain |
| 1   | A1    | 256 | ALA  | Mainchain |
| 1   | A1    | 294 | LEU  | Mainchain |
| 1   | A1    | 306 | SER  | Mainchain |
| 1   | A1    | 345 | LEU  | Mainchain |
| 1   | A1    | 383 | LEU  | Mainchain |
| 1   | A1    | 53  | ASN  | Mainchain |
| 19  | A2    | 128 | CYS  | Peptide   |
| 19  | A2    | 175 | ARG  | Peptide   |
| 19  | A2    | 308 | ARG  | Peptide   |
| 19  | A2    | 309 | ASN  | Peptide   |
| 19  | A2    | 461 | PRO  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 19  | A2    | 462 | PHE  | Peptide   |
| 2   | B1    | 106 | ALA  | Mainchain |
| 2   | B1    | 159 | VAL  | Mainchain |
| 2   | B1    | 178 | CYS  | Mainchain |
| 2   | B1    | 239 | TYR  | Mainchain |
| 2   | B1    | 285 | VAL  | Mainchain |
| 2   | B1    | 335 | ASP  | Mainchain |
| 2   | B1    | 353 | SER  | Mainchain |
| 2   | B1    | 68  | LEU  | Mainchain |
| 2   | B1    | 99  | THR  | Mainchain |
| 20  | B2    | 290 | GLY  | Peptide   |
| 20  | B2    | 291 | VAL  | Peptide   |
| 20  | B2    | 328 | ASP  | Peptide   |
| 3   | C1    | 134 | PRO  | Mainchain |
| 3   | C1    | 164 | ILE  | Mainchain |
| 3   | C1    | 20  | ASP  | Mainchain |
| 3   | C1    | 21  | LEU  | Mainchain |
| 3   | C1    | 222 | PRO  | Mainchain |
| 3   | C1    | 235 | LEU  | Mainchain |
| 3   | C1    | 281 | LEU  | Mainchain |
| 3   | C1    | 322 | GLN  | Mainchain |
| 3   | C1    | 326 | TRP  | Mainchain |
| 3   | C1    | 335 | LEU  | Mainchain |
| 3   | C1    | 355 | SER  | Mainchain |
| 3   | C1    | 362 | ILE  | Mainchain |
| 3   | C1    | 77  | TRP  | Mainchain |
| 3   | C1    | 83  | HIS  | Mainchain |
| 4   | D1    | 191 | ARG  | Mainchain |
| 4   | D1    | 217 | PRO  | Mainchain |
| 4   | D1    | 224 | ARG  | Mainchain |
| 4   | D1    | 229 | VAL  | Mainchain |
| 4   | D1    | 54  | VAL  | Mainchain |
| 22  | D2    | 161 | GLY  | Peptide   |
| 22  | D2    | 162 | TYR  | Peptide   |
| 22  | D2    | 186 | CYS  | Peptide   |
| 22  | D2    | 188 | PRO  | Peptide   |
| 5   | E1    | 20  | ASP  | Mainchain |
| 23  | E2    | 107 | PRO  | Peptide   |
| 23  | E2    | 108 | SER  | Peptide   |
| 6   | F1    | 16  | ILE  | Mainchain |
| 6   | F1    | 46  | ALA  | Mainchain |
| 7   | G1    | 15  | THR  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | G1    | 73  | ASN  | Mainchain |
| 9   | I1    | 69  | SER  | Mainchain |
| 10  | J1    | 43  | TYR  | Mainchain |
| 1   | M1    | 100 | LYS  | Mainchain |
| 1   | M1    | 141 | ASN  | Mainchain |
| 1   | M1    | 290 | LEU  | Mainchain |
| 40  | M2    | 16  | LEU  | Peptide   |
| 2   | N1    | 137 | VAL  | Mainchain |
| 2   | N1    | 144 | LEU  | Mainchain |
| 2   | N1    | 200 | THR  | Mainchain |
| 2   | N1    | 285 | VAL  | Mainchain |
| 2   | N1    | 290 | ASN  | Mainchain |
| 2   | N1    | 353 | SER  | Mainchain |
| 3   | O1    | 148 | ASN  | Mainchain |
| 3   | O1    | 159 | ASN  | Mainchain |
| 3   | O1    | 19  | ILE  | Mainchain |
| 3   | O1    | 355 | SER  | Mainchain |
| 3   | O1    | 55  | TYR  | Mainchain |
| 3   | O1    | 77  | TRP  | Mainchain |
| 4   | P1    | 202 | LYS  | Mainchain |
| 4   | P1    | 229 | VAL  | Mainchain |
| 4   | P1    | 24  | THR  | Mainchain |
| 4   | P1    | 46  | VAL  | Mainchain |
| 33  | P2    | 52  | ASN  | Peptide   |
| 5   | Q1    | 125 | GLU  | Mainchain |
| 5   | Q1    | 135 | LEU  | Mainchain |
| 5   | Q1    | 186 | GLU  | Mainchain |
| 5   | Q1    | 195 | VAL  | Mainchain |
| 5   | Q1    | 32  | ARG  | Mainchain |
| 5   | Q1    | 36  | SER  | Mainchain |
| 5   | Q1    | 49  | TYR  | Mainchain |
| 5   | Q1    | 9   | ASP  | Mainchain |
| 5   | Q1    | 97  | PHE  | Mainchain |
| 34  | Q2    | 169 | PHE  | Peptide   |
| 34  | Q2    | 91  | TYR  | Peptide   |
| 35  | R2    | 271 | TYR  | Peptide   |
| 35  | R2    | 333 | PRO  | Peptide   |
| 7   | S1    | 17  | SER  | Mainchain |
| 7   | S1    | 18  | LEU  | Mainchain |
| 7   | S1    | 34  | ILE  | Mainchain |
| 36  | S2    | 275 | ASN  | Peptide   |
| 8   | T1    | 40  | CYS  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 37  | T2    | 83  | LYS  | Peptide   |
| 9   | U1    | 72  | VAL  | Mainchain |
| 39  | V2    | 10  | MET  | Peptide   |
| 39  | V2    | 142 | TRP  | Peptide   |
| 39  | V2    | 72  | MET  | Peptide   |
| 11  | W1    | 24  | TRP  | Mainchain |
| 42  | Y2    | 89  | TYR  | Peptide   |
| 45  | b2    | 110 | TRP  | Peptide   |
| 55  | e2    | 115 | ASN  | Mainchain |
| 55  | e2    | 81  | ARG  | Peptide   |
| 55  | e2    | 87  | ASP  | Peptide   |
| 55  | e2    | 97  | LEU  | Peptide   |
| 48  | f2    | 109 | PRO  | Peptide   |
| 49  | h2    | 80  | PRO  | Peptide   |
| 49  | h2    | 81  | ALA  | Peptide   |

## 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   | A1    | 3356  | 0        | 3263     | 486     | 0            |
| 1   | M1    | 3356  | 0        | 3263     | 470     | 0            |
| 2   | B1    | 3141  | 0        | 3123     | 417     | 0            |
| 2   | N1    | 3141  | 0        | 3123     | 423     | 0            |
| 3   | C1    | 3011  | 0        | 3077     | 463     | 0            |
| 3   | O1    | 3011  | 0        | 3077     | 430     | 0            |
| 4   | D1    | 1919  | 0        | 1868     | 309     | 0            |
| 4   | P1    | 1919  | 0        | 1868     | 295     | 0            |
| 5   | E1    | 566   | 0        | 564      | 67      | 0            |
| 5   | Q1    | 1518  | 0        | 1499     | 266     | 0            |
| 6   | F1    | 916   | 0        | 911      | 96      | 0            |
| 6   | R1    | 916   | 0        | 911      | 95      | 0            |
| 7   | G1    | 682   | 0        | 679      | 108     | 0            |
| 7   | S1    | 682   | 0        | 679      | 99      | 0            |
| 8   | H1    | 524   | 0        | 504      | 69      | 0            |
| 8   | T1    | 524   | 0        | 504      | 76      | 0            |
| 9   | I1    | 248   | 0        | 265      | 53      | 0            |
| 9   | U1    | 248   | 0        | 265      | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | J1    | 511   | 0        | 518      | 73      | 0            |
| 10  | V1    | 511   | 0        | 518      | 78      | 0            |
| 11  | K1    | 164   | 0        | 161      | 29      | 0            |
| 11  | W1    | 164   | 0        | 161      | 28      | 0            |
| 12  | 22    | 2582  | 0        | 2612     | 35      | 0            |
| 13  | 32    | 719   | 0        | 741      | 9       | 0            |
| 14  | 42    | 3447  | 0        | 3442     | 48      | 0            |
| 15  | 52    | 697   | 0        | 708      | 14      | 0            |
| 16  | 72    | 1186  | 0        | 1123     | 13      | 0            |
| 17  | 82    | 2965  | 0        | 2595     | 73      | 0            |
| 18  | 92    | 1535  | 0        | 1491     | 62      | 0            |
| 19  | A2    | 5183  | 0        | 5174     | 337     | 0            |
| 20  | B2    | 3076  | 0        | 3041     | 95      | 0            |
| 21  | C2    | 1705  | 0        | 1645     | 29      | 0            |
| 22  | D2    | 1200  | 0        | 1195     | 27      | 0            |
| 23  | E2    | 1388  | 0        | 1340     | 43      | 0            |
| 24  | F2    | 183   | 0        | 132      | 6       | 0            |
| 25  | G2    | 981   | 0        | 965      | 35      | 0            |
| 26  | H2    | 780   | 0        | 753      | 12      | 0            |
| 27  | I2    | 532   | 0        | 513      | 48      | 0            |
| 28  | J2    | 530   | 0        | 503      | 7       | 0            |
| 29  | K2    | 652   | 0        | 636      | 32      | 0            |
| 30  | L2    | 602   | 0        | 592      | 9       | 0            |
| 31  | N2    | 862   | 0        | 868      | 10      | 0            |
| 32  | O2    | 925   | 0        | 907      | 9       | 0            |
| 33  | P2    | 698   | 0        | 659      | 23      | 0            |
| 34  | Q2    | 1345  | 0        | 1282     | 26      | 0            |
| 35  | R2    | 2334  | 0        | 2258     | 51      | 0            |
| 36  | S2    | 2299  | 0        | 2028     | 23      | 0            |
| 37  | T2    | 942   | 0        | 890      | 11      | 0            |
| 38  | U2    | 734   | 0        | 628      | 91      | 0            |
| 39  | V2    | 1093  | 0        | 1048     | 22      | 0            |
| 40  | M2    | 642   | 0        | 642      | 7       | 0            |
| 40  | W2    | 596   | 0        | 553      | 6       | 0            |
| 41  | X2    | 372   | 0        | 314      | 4       | 0            |
| 42  | Y2    | 409   | 0        | 318      | 7       | 0            |
| 43  | Z2    | 493   | 0        | 395      | 6       | 0            |
| 44  | a2    | 857   | 0        | 765      | 11      | 0            |
| 45  | b2    | 1032  | 0        | 954      | 14      | 0            |
| 46  | c2    | 617   | 0        | 492      | 8       | 0            |
| 47  | d2    | 708   | 0        | 514      | 9       | 0            |
| 48  | f2    | 1156  | 0        | 892      | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49  | h2    | 721   | 0        | 632      | 13      | 0            |
| 50  | i2    | 277   | 0        | 240      | 4       | 0            |
| 51  | j2    | 892   | 0        | 835      | 10      | 0            |
| 52  | l2    | 2442  | 0        | 2563     | 72      | 0            |
| 53  | 62    | 4765  | 0        | 4894     | 62      | 0            |
| 54  | g2    | 1351  | 0        | 1262     | 18      | 0            |
| 55  | e2    | 864   | 0        | 567      | 26      | 0            |
| 56  | A3    | 4025  | 0        | 4003     | 91      | 0            |
| 57  | B3    | 1822  | 0        | 1834     | 73      | 0            |
| 58  | C3    | 2124  | 0        | 2042     | 51      | 0            |
| 59  | D3    | 1195  | 0        | 1183     | 33      | 0            |
| 60  | E3    | 878   | 0        | 868      | 21      | 0            |
| 61  | F3    | 748   | 0        | 728      | 22      | 0            |
| 62  | G3    | 671   | 0        | 645      | 29      | 0            |
| 63  | H3    | 628   | 0        | 582      | 21      | 0            |
| 64  | I3    | 598   | 0        | 612      | 16      | 0            |
| 65  | J3    | 441   | 0        | 439      | 14      | 0            |
| 66  | K3    | 384   | 0        | 366      | 12      | 0            |
| 67  | L3    | 386   | 0        | 388      | 9       | 0            |
| 68  | M3    | 335   | 0        | 352      | 12      | 0            |
| 69  | C1    | 86    | 0        | 60       | 18      | 0            |
| 69  | O1    | 86    | 0        | 60       | 25      | 0            |
| 70  | D1    | 43    | 0        | 30       | 5       | 0            |
| 70  | P1    | 43    | 0        | 30       | 5       | 0            |
| 71  | 92    | 4     | 0        | 0        | 0       | 0            |
| 71  | A2    | 4     | 0        | 0        | 0       | 0            |
| 71  | Q1    | 4     | 0        | 0        | 0       | 0            |
| 72  | 22    | 41    | 0        | 59       | 3       | 0            |
| 72  | 42    | 41    | 0        | 59       | 1       | 0            |
| 72  | B2    | 51    | 0        | 82       | 1       | 0            |
| 73  | 42    | 82    | 0        | 114      | 2       | 0            |
| 74  | 82    | 31    | 0        | 19       | 2       | 0            |
| 75  | 82    | 8     | 0        | 0        | 0       | 0            |
| 75  | A2    | 16    | 0        | 0        | 12      | 0            |
| 75  | D2    | 8     | 0        | 0        | 0       | 0            |
| 75  | E2    | 16    | 0        | 0        | 0       | 0            |
| 76  | F3    | 1     | 0        | 0        | 0       | 0            |
| 76  | I2    | 1     | 0        | 0        | 1       | 0            |
| 77  | R2    | 48    | 0        | 23       | 3       | 0            |
| 78  | S2    | 47    | 0        | 71       | 0       | 0            |
| 78  | j2    | 39    | 0        | 55       | 1       | 0            |
| 79  | A3    | 120   | 0        | 108      | 4       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 80  | A3    | 1      | 0        | 0        | 0       | 0            |
| 80  | B3    | 2      | 0        | 0        | 0       | 0            |
| 81  | A3    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 105456 | 0        | 102214   | 5423    | 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 26.

All (5423) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:92:42:ARG:NH1   | 19:A2:199:GLY:HA2  | 1.33                     | 1.42              |
| 19:A2:306:MET:SD   | 38:U2:139:PRO:HG3  | 1.60                     | 1.39              |
| 52:12:126:LYS:HD3  | 52:12:127:TYR:N    | 1.31                     | 1.38              |
| 19:A2:227:PRO:HD2  | 75:A2:802:SF4:S1   | 1.63                     | 1.37              |
| 35:R2:170:LEU:O    | 35:R2:328:ILE:HD11 | 1.21                     | 1.36              |
| 19:A2:424:HIS:HA   | 25:G2:170:THR:OG1  | 1.24                     | 1.33              |
| 19:A2:422:TRP:O    | 25:G2:169:ARG:HD2  | 1.15                     | 1.31              |
| 19:A2:557:ARG:NH2  | 38:U2:144:TYR:OH   | 1.64                     | 1.30              |
| 35:R2:170:LEU:O    | 35:R2:328:ILE:CD1  | 1.78                     | 1.28              |
| 19:A2:312:GLY:HA3  | 38:U2:143:PRO:C    | 1.57                     | 1.25              |
| 77:R2:601:NAP:C1D  | 77:R2:601:NAP:O4D  | 1.63                     | 1.24              |
| 52:12:75:PRO:HG3   | 52:12:223:PHE:CZ   | 1.74                     | 1.22              |
| 9:I1:72:VAL:HB     | 9:I1:73:PRO:HD3    | 1.20                     | 1.20              |
| 19:A2:312:GLY:O    | 38:U2:141:SER:O    | 1.61                     | 1.18              |
| 7:S1:50:PRO:HB2    | 7:S1:51:PRO:HD3    | 1.25                     | 1.17              |
| 4:D1:224:ARG:HB2   | 7:G1:25:ALA:HB1    | 1.27                     | 1.17              |
| 19:A2:314:LEU:CD2  | 38:U2:140:PRO:HD2  | 1.74                     | 1.17              |
| 7:G1:72:LYS:HB3    | 7:G1:75:ALA:HB2    | 1.19                     | 1.16              |
| 2:B1:77:THR:HG22   | 2:B1:130:PRO:HA    | 1.25                     | 1.15              |
| 19:A2:312:GLY:HA3  | 38:U2:143:PRO:O    | 0.97                     | 1.15              |
| 5:Q1:114:VAL:HA    | 5:Q1:117:LEU:HD12  | 1.24                     | 1.14              |
| 1:M1:426:GLY:CA    | 1:M1:428:ILE:HG13  | 1.78                     | 1.14              |
| 11:W1:29:ALA:O     | 11:W1:33:VAL:HG23  | 1.46                     | 1.14              |
| 55:e2:36:MET:HA    | 55:e2:77:LYS:CE    | 1.78                     | 1.13              |
| 1:A1:428:ILE:HG22  | 1:A1:431:LEU:HB2   | 1.29                     | 1.13              |
| 19:A2:312:GLY:CA   | 38:U2:143:PRO:O    | 1.94                     | 1.13              |
| 1:M1:67:THR:HG23   | 1:M1:70:ARG:H      | 1.13                     | 1.13              |
| 2:B1:60:SER:HB3    | 2:N1:429:ASN:HD21  | 0.96                     | 1.12              |
| 4:P1:83:ARG:HB3    | 4:P1:84:PRO:HD2    | 1.14                     | 1.12              |
| 35:R2:328:ILE:HG22 | 35:R2:329:LEU:H    | 1.09                     | 1.12              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:428:ILE:HG22  | 1:M1:431:LEU:HB2   | 1.19                     | 1.11              |
| 19:A2:422:TRP:O    | 25:G2:169:ARG:CD   | 1.99                     | 1.11              |
| 3:C1:129:MET:HG2   | 3:C1:178:PHE:HD2   | 1.03                     | 1.11              |
| 4:P1:83:ARG:HB3    | 4:P1:84:PRO:CD     | 1.81                     | 1.10              |
| 18:92:42:ARG:CZ    | 19:A2:199:GLY:HA2  | 1.80                     | 1.10              |
| 55:e2:36:MET:HA    | 55:e2:77:LYS:HE3   | 1.11                     | 1.10              |
| 5:Q1:15:ARG:HB2    | 5:Q1:16:PRO:HD2    | 1.19                     | 1.10              |
| 19:A2:557:ARG:CZ   | 38:U2:144:TYR:OH   | 1.99                     | 1.09              |
| 17:82:225:LEU:CD2  | 19:A2:93:ALA:HB3   | 1.80                     | 1.09              |
| 1:M1:428:ILE:HG21  | 1:M1:431:LEU:HD22  | 1.35                     | 1.09              |
| 3:C1:77:TRP:CZ3    | 3:C1:78:ILE:HG23   | 1.88                     | 1.08              |
| 1:M1:403:ASP:HB3   | 1:M1:406:VAL:HG23  | 1.34                     | 1.08              |
| 36:S2:200:PRO:HG3  | 36:S2:223:GLN:HE22 | 1.17                     | 1.08              |
| 11:W1:30:VAL:O     | 11:W1:34:TRP:CD1   | 2.05                     | 1.08              |
| 5:Q1:76:ILE:CG2    | 5:Q1:194:ILE:HG12  | 1.84                     | 1.08              |
| 19:A2:144:MET:HA   | 20:B2:380:HIS:NE2  | 1.68                     | 1.08              |
| 4:P1:181:GLN:HG2   | 8:T1:77:LEU:HD22   | 1.29                     | 1.07              |
| 18:92:124:ARG:NH1  | 19:A2:209:TYR:OH   | 1.87                     | 1.07              |
| 19:A2:161:GLU:N    | 27:I2:102:ASN:HD22 | 1.52                     | 1.07              |
| 20:B2:94:VAL:HG12  | 20:B2:115:LEU:HD22 | 1.27                     | 1.07              |
| 3:O1:26:ASN:HD21   | 3:O1:207:ASN:HB2   | 1.15                     | 1.07              |
| 3:O1:206:ASN:HB2   | 3:O1:313:ARG:NH2   | 1.68                     | 1.07              |
| 18:92:95:ILE:HD11  | 19:A2:210:ILE:CG2  | 1.84                     | 1.07              |
| 3:C1:206:ASN:HB2   | 3:C1:313:ARG:NH2   | 1.70                     | 1.07              |
| 1:A1:41:ILE:HG13   | 1:A1:195:MET:HE3   | 1.36                     | 1.06              |
| 9:U1:72:VAL:HB     | 9:U1:73:PRO:HD3    | 1.36                     | 1.06              |
| 1:A1:67:THR:HG23   | 1:A1:70:ARG:H      | 0.94                     | 1.06              |
| 19:A2:314:LEU:HD23 | 38:U2:140:PRO:HD2  | 1.09                     | 1.06              |
| 1:M1:24:ARG:HB2    | 1:M1:196:VAL:HG22  | 1.37                     | 1.06              |
| 2:N1:200:THR:HG22  | 2:N1:203:ARG:HD2   | 1.36                     | 1.06              |
| 55:e2:75:TYR:HB3   | 55:e2:78:LEU:CB    | 1.83                     | 1.06              |
| 1:A1:64:PHE:CE1    | 1:A1:86:LEU:HG     | 1.90                     | 1.05              |
| 3:C1:310:SER:HA    | 3:C1:374:ASN:HD21  | 1.12                     | 1.05              |
| 2:N1:305:GLN:HB2   | 2:N1:306:PRO:HD3   | 1.34                     | 1.05              |
| 3:O1:310:SER:HA    | 3:O1:374:ASN:HD21  | 1.21                     | 1.05              |
| 9:I1:72:VAL:HB     | 9:I1:73:PRO:CD     | 1.86                     | 1.05              |
| 5:Q1:96:LEU:HD21   | 5:Q1:195:VAL:HG21  | 1.38                     | 1.05              |
| 17:82:418:GLN:HE21 | 19:A2:115:GLY:CA   | 1.70                     | 1.05              |
| 5:Q1:109:GLU:HG2   | 5:Q1:167:ALA:HB3   | 1.37                     | 1.04              |
| 1:A1:18:GLN:HE21   | 1:A1:22:GLY:HA2    | 1.19                     | 1.04              |
| 4:D1:181:GLN:HG2   | 8:H1:77:LEU:HD22   | 1.40                     | 1.04              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:426:GLY:CA    | 1:A1:428:ILE:HG13  | 1.87                     | 1.04              |
| 3:C1:170:VAL:HG13  | 3:C1:174:THR:HG21  | 1.34                     | 1.04              |
| 7:G1:34:ILE:HB     | 7:G1:35:PRO:HD3    | 1.39                     | 1.04              |
| 7:S1:72:LYS:HB3    | 7:S1:75:ALA:HB2    | 1.39                     | 1.04              |
| 3:C1:129:MET:HG2   | 3:C1:178:PHE:CD2   | 1.93                     | 1.04              |
| 4:D1:83:ARG:HB3    | 4:D1:84:PRO:CD     | 1.86                     | 1.04              |
| 5:Q1:75:GLU:O      | 5:Q1:194:ILE:HA    | 1.57                     | 1.04              |
| 2:B1:283:PRO:HG3   | 9:I1:55:LEU:HD22   | 1.39                     | 1.03              |
| 2:B1:429:ASN:HD21  | 2:N1:60:SER:HB3    | 1.15                     | 1.03              |
| 20:B2:82:LEU:HD21  | 52:12:126:LYS:HG3  | 1.04                     | 1.03              |
| 2:B1:24:LEU:H      | 2:B1:24:LEU:HD12   | 1.23                     | 1.03              |
| 5:Q1:134:ILE:HD11  | 5:Q1:185:TYR:CD2   | 1.94                     | 1.03              |
| 10:J1:18:SER:HB3   | 11:K1:23:LEU:HD12  | 1.42                     | 1.02              |
| 52:12:75:PRO:CG    | 52:12:223:PHE:CZ   | 2.42                     | 1.02              |
| 2:B1:95:LYS:HE3    | 9:I1:70:LEU:HD22   | 1.41                     | 1.02              |
| 3:C1:202:GLU:OE2   | 3:O1:10:LEU:HB2    | 1.59                     | 1.02              |
| 47:d2:25:PHE:CD2   | 47:d2:40:VAL:CB    | 2.42                     | 1.02              |
| 6:R1:28:LYS:HD2    | 6:R1:74:ILE:HD11   | 1.42                     | 1.01              |
| 19:A2:161:GLU:HB3  | 27:I2:102:ASN:ND2  | 1.74                     | 1.01              |
| 3:C1:16:ASN:ND2    | 3:C1:20:ASP:OD2    | 1.93                     | 1.01              |
| 1:M1:428:ILE:HG22  | 1:M1:431:LEU:CB    | 1.91                     | 1.01              |
| 2:B1:165:ALA:HA    | 2:B1:173:ALA:HB1   | 1.39                     | 1.01              |
| 4:P1:224:ARG:HB2   | 7:S1:25:ALA:HB1    | 1.40                     | 1.01              |
| 2:B1:60:SER:CB     | 2:N1:429:ASN:HD21  | 1.72                     | 1.01              |
| 3:C1:221:HIS:HB3   | 3:C1:222:PRO:HD3   | 1.42                     | 1.00              |
| 3:O1:174:THR:HG23  | 3:O1:178:PHE:HE2   | 1.25                     | 1.00              |
| 2:B1:52:LYS:HB2    | 2:B1:203:ARG:HB3   | 1.39                     | 1.00              |
| 17:82:225:LEU:HD22 | 19:A2:93:ALA:HB3   | 1.04                     | 1.00              |
| 1:M1:18:GLN:HE21   | 1:M1:22:GLY:HA2    | 1.23                     | 1.00              |
| 2:N1:166:ALA:HB2   | 2:N1:244:ILE:HG13  | 1.39                     | 1.00              |
| 52:12:126:LYS:CD   | 52:12:127:TYR:N    | 2.24                     | 1.00              |
| 19:A2:312:GLY:CA   | 38:U2:143:PRO:C    | 2.31                     | 1.00              |
| 4:D1:74:PRO:HB2    | 4:D1:79:GLU:HB2    | 1.43                     | 1.00              |
| 3:C1:100:ARG:HH21  | 69:C1:402:HEM:HBD1 | 1.26                     | 1.00              |
| 4:D1:83:ARG:HB3    | 4:D1:84:PRO:HD2    | 1.00                     | 0.99              |
| 4:D1:83:ARG:CB     | 4:D1:84:PRO:HD2    | 1.90                     | 0.99              |
| 3:C1:206:ASN:HB2   | 3:C1:313:ARG:HH21  | 1.24                     | 0.99              |
| 1:M1:143:THR:HG21  | 9:U1:48:SER:H      | 1.24                     | 0.99              |
| 3:C1:264:THR:HG21  | 5:Q1:144:CYS:HB3   | 1.44                     | 0.99              |
| 3:C1:10:LEU:HB2    | 3:O1:202:GLU:OE2   | 1.59                     | 0.99              |
| 3:C1:26:ASN:HB2    | 6:F1:69:SER:OG     | 1.62                     | 0.99              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:100:ARG:HH21  | 69:O1:402:HEM:HBD1 | 1.23                     | 0.99              |
| 17:82:418:GLN:NE2  | 19:A2:115:GLY:HA2  | 1.77                     | 0.99              |
| 19:A2:613:PRO:CB   | 38:U2:134:ILE:HG21 | 1.91                     | 0.99              |
| 1:M1:64:PHE:CE1    | 1:M1:86:LEU:HG     | 1.98                     | 0.99              |
| 9:U1:70:LEU:HD21   | 9:U1:73:PRO:HD2    | 1.40                     | 0.99              |
| 3:O1:16:ASN:ND2    | 3:O1:20:ASP:OD2    | 1.96                     | 0.99              |
| 5:Q1:86:ASN:HB2    | 5:Q1:99:ARG:HD2    | 1.45                     | 0.99              |
| 8:T1:21:ARG:HB3    | 8:T1:65:ARG:HH21   | 1.26                     | 0.99              |
| 17:82:225:LEU:HD22 | 19:A2:93:ALA:CB    | 1.92                     | 0.99              |
| 4:D1:118:ARG:HG3   | 4:D1:194:ALA:HB1   | 1.44                     | 0.98              |
| 1:A1:408:ARG:HH22  | 11:K1:15:ARG:NE    | 1.61                     | 0.98              |
| 3:C1:179:PHE:HE2   | 3:O1:179:PHE:HE2   | 1.05                     | 0.98              |
| 20:B2:82:LEU:CD2   | 52:12:126:LYS:HG3  | 1.93                     | 0.98              |
| 6:F1:51:PRO:HG2    | 6:F1:54:LEU:HD23   | 1.44                     | 0.98              |
| 52:12:75:PRO:HA    | 52:12:223:PHE:HE1  | 1.26                     | 0.98              |
| 2:B1:200:THR:HG22  | 2:B1:203:ARG:HD2   | 1.44                     | 0.98              |
| 2:B1:429:ASN:HD21  | 2:N1:60:SER:CB     | 1.74                     | 0.98              |
| 17:82:383:THR:HG23 | 19:A2:75:CYS:HA    | 1.45                     | 0.98              |
| 1:M1:417:ASP:OD2   | 10:V1:10:TYR:OH    | 1.82                     | 0.98              |
| 4:P1:74:PRO:HB2    | 4:P1:79:GLU:HB2    | 1.46                     | 0.98              |
| 19:A2:613:PRO:HB3  | 38:U2:134:ILE:HG21 | 1.45                     | 0.98              |
| 2:N1:111:CYS:HB3   | 2:N1:119:LEU:HD22  | 1.46                     | 0.98              |
| 20:B2:82:LEU:HD21  | 52:12:126:LYS:CG   | 1.93                     | 0.98              |
| 1:A1:383:LEU:HD22  | 1:A1:388:ARG:HA    | 1.45                     | 0.98              |
| 2:B1:24:LEU:HG     | 2:B1:38:LEU:HD11   | 1.42                     | 0.98              |
| 1:A1:304:CYS:HB3   | 1:A1:334:MET:SD    | 2.04                     | 0.97              |
| 3:C1:174:THR:HG23  | 3:C1:178:PHE:CE1   | 1.98                     | 0.97              |
| 3:O1:345:HIS:HB3   | 3:O1:346:PRO:HD3   | 1.42                     | 0.97              |
| 1:A1:343:MET:HE1   | 1:A1:416:TYR:CD2   | 1.98                     | 0.97              |
| 55:e2:70:THR:O     | 55:e2:72:TYR:N     | 1.96                     | 0.97              |
| 70:P1:301:HEC:HHD  | 70:P1:301:HEC:HBC2 | 1.45                     | 0.97              |
| 1:M1:408:ARG:HH22  | 11:W1:15:ARG:NE    | 1.61                     | 0.97              |
| 2:N1:24:LEU:HG     | 2:N1:38:LEU:HD11   | 1.43                     | 0.97              |
| 4:P1:158:ILE:CD1   | 4:P1:160:MET:HB2   | 1.94                     | 0.97              |
| 18:92:42:ARG:NH1   | 19:A2:199:GLY:CA   | 2.27                     | 0.97              |
| 1:A1:24:ARG:HB2    | 1:A1:196:VAL:HG22  | 1.43                     | 0.97              |
| 1:A1:403:ASP:HB3   | 1:A1:406:VAL:HG23  | 1.46                     | 0.97              |
| 1:M1:392:LEU:HA    | 1:M1:395:TRP:CD1   | 1.99                     | 0.97              |
| 1:M1:42:ASP:HB3    | 1:M1:384:LEU:HD22  | 1.45                     | 0.97              |
| 18:92:110:MET:SD   | 19:A2:194:ASP:O    | 2.23                     | 0.97              |
| 3:O1:77:TRP:CZ3    | 3:O1:78:ILE:HG23   | 1.98                     | 0.96              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:A2:302:LEU:HA   | 38:U2:137:TRP:CB   | 1.95                     | 0.96              |
| 2:N1:283:PRO:HG3   | 9:U1:55:LEU:HD22   | 1.47                     | 0.96              |
| 2:B1:67:HIS:HD2    | 2:B1:144:LEU:HD22  | 1.27                     | 0.96              |
| 1:A1:67:THR:HG23   | 1:A1:70:ARG:N      | 1.79                     | 0.96              |
| 3:C1:26:ASN:HD21   | 3:C1:207:ASN:HB2   | 1.28                     | 0.96              |
| 6:F1:50:LEU:HB2    | 6:F1:55:TYR:HB2    | 1.45                     | 0.96              |
| 27:I2:104:ASP:O    | 27:I2:105:LYS:HB3  | 1.63                     | 0.96              |
| 3:O1:106:SER:HB3   | 69:O1:402:HEM:HBD2 | 1.46                     | 0.96              |
| 3:C1:115:ILE:HG21  | 3:C1:196:HIS:HB2   | 1.48                     | 0.95              |
| 9:I1:70:LEU:HD21   | 9:I1:73:PRO:HD2    | 1.48                     | 0.95              |
| 7:G1:36:ASN:HA     | 7:G1:39:ARG:HD3    | 1.46                     | 0.95              |
| 2:B1:60:SER:HB3    | 2:N1:429:ASN:ND2   | 1.81                     | 0.95              |
| 18:92:42:ARG:HH12  | 19:A2:199:GLY:HA2  | 1.23                     | 0.95              |
| 19:A2:313:LEU:CD2  | 38:U2:142:THR:CB   | 2.43                     | 0.95              |
| 17:82:383:THR:CG2  | 19:A2:75:CYS:HA    | 1.95                     | 0.95              |
| 20:B2:94:VAL:HG12  | 20:B2:115:LEU:CD2  | 1.96                     | 0.95              |
| 7:S1:31:SER:O      | 7:S1:35:PRO:HD2    | 1.65                     | 0.95              |
| 2:B1:304:HIS:CD2   | 2:B1:306:PRO:HD2   | 2.01                     | 0.95              |
| 52:12:75:PRO:HA    | 52:12:223:PHE:CE1  | 2.02                     | 0.95              |
| 2:B1:305:GLN:HB2   | 2:B1:306:PRO:HD3   | 1.46                     | 0.95              |
| 2:N1:51:ILE:HG21   | 2:N1:199:PHE:HA    | 1.48                     | 0.95              |
| 20:B2:97:LEU:H     | 20:B2:97:LEU:HD12  | 1.31                     | 0.95              |
| 2:B1:159:VAL:HG12  | 2:B1:160:ILE:HD13  | 1.48                     | 0.95              |
| 3:O1:210:GLY:HA3   | 3:O1:314:SER:HB2   | 1.46                     | 0.95              |
| 2:N1:77:THR:HG22   | 2:N1:130:PRO:HA    | 1.46                     | 0.95              |
| 3:O1:174:THR:HG23  | 3:O1:178:PHE:CE2   | 2.00                     | 0.95              |
| 1:M1:61:HIS:NE2    | 1:M1:134:ILE:HD11  | 1.82                     | 0.94              |
| 2:B1:51:ILE:HG21   | 2:B1:199:PHE:HA    | 1.49                     | 0.94              |
| 35:R2:328:ILE:CG2  | 35:R2:329:LEU:H    | 1.80                     | 0.94              |
| 56:A3:365:ILE:HD12 | 57:B3:87:MET:HE1   | 1.48                     | 0.94              |
| 3:O1:108:THR:HB    | 3:O1:313:ARG:HH11  | 1.31                     | 0.94              |
| 4:P1:158:ILE:HD13  | 4:P1:160:MET:HB2   | 1.49                     | 0.94              |
| 1:M1:21:ASN:HB3    | 1:M1:217:SER:HB3   | 1.46                     | 0.94              |
| 4:P1:178:THR:HB    | 4:P1:181:GLN:HG3   | 1.46                     | 0.94              |
| 1:A1:61:HIS:CD2    | 1:A1:134:ILE:HD11  | 2.03                     | 0.94              |
| 3:C1:240:MET:HA    | 3:C1:243:VAL:HG12  | 1.49                     | 0.94              |
| 3:C1:310:SER:HB3   | 3:C1:318:ARG:NH1   | 1.82                     | 0.94              |
| 19:A2:527:ASP:O    | 29:K2:56:ARG:NH2   | 2.01                     | 0.94              |
| 7:G1:9:ARG:NH2     | 7:G1:11:ARG:HD2    | 1.83                     | 0.94              |
| 2:N1:248:ASN:HB2   | 2:N1:428:GLY:HA2   | 1.46                     | 0.94              |
| 3:O1:252:ASP:HB3   | 3:O1:253:PRO:HD3   | 1.50                     | 0.94              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:H1:50:THR:HG22   | 8:H1:52:GLU:H     | 1.28                     | 0.94              |
| 2:N1:67:HIS:HD2    | 2:N1:144:LEU:HD22 | 1.30                     | 0.94              |
| 4:D1:165:TYR:O     | 4:D1:168:VAL:HG23 | 1.67                     | 0.94              |
| 19:A2:674:LEU:HD12 | 29:K2:46:LYS:HE2  | 1.49                     | 0.94              |
| 3:C1:174:THR:HG23  | 3:C1:178:PHE:HE1  | 1.31                     | 0.93              |
| 5:Q1:85:LYS:HG2    | 5:Q1:86:ASN:H     | 1.33                     | 0.93              |
| 2:N1:29:LEU:HB3    | 2:N1:30:PRO:HD2   | 1.48                     | 0.93              |
| 2:N1:132:PHE:CD2   | 2:N1:191:LEU:HD13 | 2.04                     | 0.93              |
| 3:O1:135:TRP:HH2   | 3:O1:170:VAL:HG12 | 1.32                     | 0.93              |
| 9:U1:72:VAL:HB     | 9:U1:73:PRO:CD    | 1.98                     | 0.93              |
| 62:G3:5:LYS:HZ3    | 62:G3:6:GLY:H     | 1.02                     | 0.93              |
| 1:A1:133:VAL:HG12  | 1:A1:134:ILE:HD13 | 1.48                     | 0.93              |
| 1:A1:67:THR:CG2    | 1:A1:70:ARG:H     | 1.81                     | 0.93              |
| 19:A2:557:ARG:NE   | 38:U2:144:TYR:OH  | 2.01                     | 0.93              |
| 19:A2:306:MET:SD   | 38:U2:139:PRO:CG  | 2.56                     | 0.93              |
| 2:N1:316:TYR:OH    | 9:U1:64:LEU:HD23  | 1.67                     | 0.93              |
| 17:82:418:GLN:HE21 | 19:A2:115:GLY:HA2 | 1.30                     | 0.92              |
| 1:A1:346:CYS:HB3   | 1:A1:412:SER:OG   | 1.68                     | 0.92              |
| 1:A1:144:SER:O     | 1:A1:148:VAL:HG23 | 1.69                     | 0.92              |
| 2:B1:77:THR:HG22   | 2:B1:130:PRO:CA   | 1.99                     | 0.92              |
| 2:N1:207:ILE:HD11  | 2:N1:383:GLY:HA2  | 1.49                     | 0.92              |
| 19:A2:161:GLU:OE1  | 27:I2:102:ASN:ND2 | 2.00                     | 0.92              |
| 56:A3:449:MET:SD   | 57:B3:5:MET:HE2   | 2.09                     | 0.92              |
| 1:A1:91:THR:HG22   | 1:A1:93:GLU:H     | 1.35                     | 0.92              |
| 2:B1:111:CYS:HB3   | 2:B1:119:LEU:HD22 | 1.49                     | 0.92              |
| 2:B1:385:GLN:HG2   | 9:I1:62:ARG:HH12  | 1.35                     | 0.92              |
| 1:M1:61:HIS:CE1    | 1:M1:134:ILE:HD11 | 2.04                     | 0.92              |
| 1:A1:417:ASP:OD2   | 10:J1:10:TYR:OH   | 1.88                     | 0.91              |
| 3:O1:26:ASN:ND2    | 3:O1:207:ASN:HB2  | 1.85                     | 0.91              |
| 1:M1:91:THR:HG22   | 1:M1:93:GLU:H     | 1.32                     | 0.91              |
| 1:A1:392:LEU:HA    | 1:A1:395:TRP:CD1  | 2.05                     | 0.91              |
| 4:D1:74:PRO:HG2    | 4:D1:82:MET:SD    | 2.10                     | 0.91              |
| 4:P1:23:HIS:HA     | 4:P1:26:ILE:HD12  | 1.49                     | 0.91              |
| 5:Q1:15:ARG:HH21   | 5:Q1:32:ARG:HG3   | 1.35                     | 0.91              |
| 5:Q1:109:GLU:CG    | 5:Q1:167:ALA:HB3  | 2.01                     | 0.91              |
| 2:B1:162:ASN:HD22  | 2:B1:244:ILE:CG2  | 1.83                     | 0.91              |
| 17:82:381:GLN:O    | 19:A2:74:ASN:HB2  | 1.70                     | 0.91              |
| 19:A2:424:HIS:CA   | 25:G2:170:THR:OG1 | 2.17                     | 0.90              |
| 19:A2:266:ARG:NH2  | 23:E2:130:ILE:O   | 2.05                     | 0.90              |
| 1:A1:69:ASN:O      | 1:A1:71:PRO:HD3   | 1.70                     | 0.90              |
| 1:A1:143:THR:HG21  | 9:I1:48:SER:H     | 1.33                     | 0.90              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:12:75:PRO:CD   | 52:12:223:PHE:HZ   | 1.85                     | 0.90              |
| 3:C1:34:GLY:O     | 3:C1:37:LEU:HB2    | 1.72                     | 0.90              |
| 2:B1:29:LEU:HB3   | 2:B1:30:PRO:HD2    | 1.54                     | 0.90              |
| 19:A2:129:PRO:HD2 | 27:I2:114:TYR:OH   | 1.70                     | 0.90              |
| 2:B1:342:ASN:O    | 2:B1:345:LYS:HB2   | 1.72                     | 0.90              |
| 3:C1:252:ASP:HB3  | 3:C1:253:PRO:HD3   | 1.52                     | 0.90              |
| 3:O1:122:THR:HG22 | 3:O1:189:ILE:HD11  | 1.51                     | 0.90              |
| 3:O1:206:ASN:HB2  | 3:O1:313:ARG:HH21  | 1.28                     | 0.90              |
| 5:Q1:15:ARG:NH2   | 5:Q1:32:ARG:HG3    | 1.87                     | 0.90              |
| 17:82:390:ASP:OD2 | 19:A2:202:ASN:HB2  | 1.70                     | 0.89              |
| 1:M1:383:LEU:HD22 | 1:M1:388:ARG:HA    | 1.54                     | 0.89              |
| 3:O1:221:HIS:HB3  | 3:O1:222:PRO:HD3   | 1.52                     | 0.89              |
| 2:B1:258:VAL:HG11 | 2:B1:321:LEU:HB3   | 1.53                     | 0.89              |
| 4:D1:178:THR:OG1  | 4:D1:181:GLN:NE2   | 2.05                     | 0.89              |
| 6:F1:47:ILE:O     | 6:F1:50:LEU:HG     | 1.72                     | 0.89              |
| 18:92:110:MET:HE2 | 19:A2:195:LEU:C    | 1.96                     | 0.89              |
| 3:C1:103:TYR:HA   | 3:C1:315:MET:HE3   | 1.52                     | 0.89              |
| 4:P1:165:TYR:O    | 4:P1:168:VAL:HG23  | 1.73                     | 0.89              |
| 19:A2:137:CYS:HB3 | 75:A2:801:SF4:S4   | 2.12                     | 0.89              |
| 19:A2:424:HIS:HA  | 25:G2:170:THR:HG1  | 1.32                     | 0.89              |
| 52:12:126:LYS:HD3 | 52:12:127:TYR:H    | 1.11                     | 0.89              |
| 1:A1:236:PHE:CE2  | 1:A1:258:GLU:HB3   | 2.07                     | 0.89              |
| 4:D1:231:LYS:HD2  | 6:F1:71:ARG:HG2    | 1.52                     | 0.89              |
| 1:A1:426:GLY:H    | 1:A1:428:ILE:CG1   | 1.85                     | 0.89              |
| 3:C1:266:PRO:HB3  | 5:Q1:160:CYS:HA    | 1.54                     | 0.89              |
| 1:M1:236:PHE:CE2  | 1:M1:258:GLU:HB3   | 2.07                     | 0.89              |
| 7:S1:50:PRO:HB2   | 7:S1:51:PRO:CD     | 2.03                     | 0.89              |
| 1:M1:158:PHE:CE1  | 1:M1:317:THR:HG21  | 2.08                     | 0.89              |
| 2:N1:52:LYS:HB2   | 2:N1:203:ARG:HB3   | 1.54                     | 0.89              |
| 19:A2:302:LEU:CA  | 38:U2:137:TRP:HB2  | 2.03                     | 0.89              |
| 1:A1:40:TRP:CZ2   | 1:A1:377:GLU:HA    | 2.08                     | 0.88              |
| 7:S1:9:ARG:NH2    | 7:S1:11:ARG:HD2    | 1.87                     | 0.88              |
| 1:M1:45:SER:HB3   | 1:M1:92:ARG:HA     | 1.53                     | 0.88              |
| 2:N1:385:GLN:HG2  | 9:U1:62:ARG:HH12   | 1.38                     | 0.88              |
| 8:H1:73:LEU:HD23  | 8:H1:74:PHE:N      | 1.89                     | 0.88              |
| 4:D1:176:PRO:HB2  | 4:D1:181:GLN:HE22  | 1.37                     | 0.88              |
| 3:O1:361:LEU:HD23 | 3:O1:365:LEU:HD12  | 1.54                     | 0.88              |
| 20:B2:91:ALA:HB2  | 20:B2:193:ASP:OD2  | 1.73                     | 0.88              |
| 22:D2:114:ARG:HG3 | 22:D2:114:ARG:HH21 | 1.39                     | 0.88              |
| 1:A1:408:ARG:NH1  | 11:K1:15:ARG:HE    | 1.71                     | 0.88              |
| 2:B1:406:ALA:HB3  | 2:B1:409:ASP:HB2   | 1.53                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:A2:182:CYS:N    | 75:A2:802:SF4:S2   | 2.47                     | 0.88              |
| 18:92:42:ARG:NH2   | 19:A2:203:ASP:O    | 2.07                     | 0.88              |
| 1:A1:156:THR:HG23  | 1:A1:239:SER:OG    | 1.73                     | 0.88              |
| 2:N1:123:LEU:O     | 2:N1:127:THR:HG22  | 1.74                     | 0.88              |
| 4:P1:118:ARG:HG3   | 4:P1:194:ALA:HB1   | 1.55                     | 0.88              |
| 52:12:25:ARG:HG2   | 52:12:25:ARG:HH11  | 1.36                     | 0.88              |
| 1:A1:343:MET:HE1   | 1:A1:416:TYR:HD2   | 1.33                     | 0.87              |
| 1:M1:426:GLY:HA3   | 1:M1:428:ILE:HG13  | 1.54                     | 0.87              |
| 2:N1:304:HIS:CD2   | 2:N1:306:PRO:HD2   | 2.08                     | 0.87              |
| 35:R2:328:ILE:HG22 | 35:R2:329:LEU:N    | 1.80                     | 0.87              |
| 3:C1:179:PHE:CE2   | 3:O1:179:PHE:HE2   | 1.92                     | 0.87              |
| 3:C1:185:LEU:HB3   | 3:C1:186:PRO:HD3   | 1.55                     | 0.87              |
| 11:K1:29:ALA:O     | 11:K1:33:VAL:HG12  | 1.73                     | 0.87              |
| 18:92:95:ILE:CD1   | 19:A2:210:ILE:CG2  | 2.53                     | 0.87              |
| 58:C3:112:LEU:HG   | 58:C3:118:PRO:HB3  | 1.55                     | 0.87              |
| 19:A2:313:LEU:HD21 | 38:U2:142:THR:CB   | 2.05                     | 0.87              |
| 5:E1:15:ARG:HB2    | 5:E1:16:PRO:HD2    | 1.57                     | 0.87              |
| 1:A1:260:PRO:HD3   | 1:A1:414:TYR:CE1   | 2.10                     | 0.87              |
| 2:N1:305:GLN:HB2   | 2:N1:306:PRO:CD    | 2.05                     | 0.87              |
| 3:O1:108:THR:HB    | 3:O1:313:ARG:NH1   | 1.89                     | 0.87              |
| 2:N1:347:ILE:O     | 2:N1:411:ILE:HG23  | 1.75                     | 0.86              |
| 5:Q1:15:ARG:HB2    | 5:Q1:16:PRO:CD     | 2.02                     | 0.86              |
| 3:C1:6:LYS:HE2     | 3:C1:16:ASN:HD21   | 1.38                     | 0.86              |
| 3:C1:170:VAL:HG13  | 3:C1:174:THR:CG2   | 2.04                     | 0.86              |
| 3:C1:179:PHE:HE2   | 3:O1:179:PHE:CE2   | 1.92                     | 0.86              |
| 1:M1:408:ARG:HH12  | 11:W1:15:ARG:HE    | 1.20                     | 0.86              |
| 3:O1:334:THR:O     | 3:O1:338:ILE:HD13  | 1.75                     | 0.86              |
| 10:J1:58:LYS:HG2   | 10:J1:59:TYR:H     | 1.41                     | 0.86              |
| 5:Q1:118:ARG:HH11  | 5:Q1:171:ILE:CG1   | 1.88                     | 0.86              |
| 5:Q1:60:SER:HA     | 5:Q1:63:SER:OG     | 1.75                     | 0.86              |
| 17:82:424:ILE:HG12 | 19:A2:76:ARG:NH2   | 1.89                     | 0.86              |
| 1:M1:408:ARG:NH1   | 11:W1:15:ARG:HE    | 1.73                     | 0.86              |
| 7:S1:36:ASN:HA     | 7:S1:39:ARG:HD3    | 1.57                     | 0.86              |
| 35:R2:170:LEU:O    | 35:R2:328:ILE:HD12 | 1.73                     | 0.86              |
| 2:N1:209:LEU:HD22  | 2:N1:375:SER:HB2   | 1.56                     | 0.85              |
| 3:C1:10:LEU:HD12   | 3:C1:13:ILE:HD11   | 1.55                     | 0.85              |
| 1:M1:213:GLN:HB3   | 1:M1:215:HIS:NE2   | 1.91                     | 0.85              |
| 1:M1:52:ASN:HB2    | 1:M1:55:ALA:HB2    | 1.58                     | 0.85              |
| 1:A1:213:GLN:HB3   | 1:A1:215:HIS:NE2   | 1.91                     | 0.85              |
| 9:I1:70:LEU:CD2    | 9:I1:73:PRO:HD2    | 2.07                     | 0.85              |
| 1:M1:343:MET:HE1   | 1:M1:416:TYR:CD2   | 2.10                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:R1:75:LEU:HD12  | 6:R1:76:PRO:HD2    | 1.57                     | 0.85              |
| 10:V1:29:LEU:HD13 | 11:W1:34:TRP:HB3   | 1.58                     | 0.85              |
| 19:A2:67:GLU:O    | 25:G2:158:LYS:NZ   | 2.09                     | 0.85              |
| 52:12:126:LYS:HD3 | 52:12:127:TYR:CA   | 2.07                     | 0.85              |
| 18:92:95:ILE:CD1  | 19:A2:210:ILE:HG22 | 2.07                     | 0.85              |
| 1:A1:46:ARG:HH22  | 1:A1:316:ASP:CG    | 1.83                     | 0.85              |
| 1:A1:64:PHE:HE1   | 1:A1:86:LEU:HG     | 1.36                     | 0.85              |
| 18:92:224:SER:OG  | 18:92:226:GLU:HG2  | 1.75                     | 0.85              |
| 19:A2:227:PRO:CD  | 75:A2:802:SF4:S1   | 2.59                     | 0.85              |
| 18:92:42:ARG:CZ   | 19:A2:199:GLY:CA   | 2.55                     | 0.85              |
| 9:I1:72:VAL:CB    | 9:I1:73:PRO:HD3    | 2.05                     | 0.85              |
| 2:N1:263:ALA:O    | 2:N1:269:ALA:HB2   | 1.77                     | 0.85              |
| 3:O1:30:TRP:O     | 3:O1:33:PHE:HD2    | 1.59                     | 0.85              |
| 3:O1:234:LEU:HD23 | 4:P1:216:LEU:HD21  | 1.59                     | 0.84              |
| 5:Q1:187:PHE:CD2  | 5:Q1:193:VAL:HB    | 2.11                     | 0.84              |
| 2:B1:286:LYS:HD3  | 2:B1:287:ARG:NH1   | 1.92                     | 0.84              |
| 7:S1:34:ILE:HB    | 7:S1:35:PRO:HD3    | 1.58                     | 0.84              |
| 19:A2:312:GLY:C   | 38:U2:141:SER:O    | 2.19                     | 0.84              |
| 1:A1:21:ASN:HB3   | 1:A1:217:SER:CB    | 2.07                     | 0.84              |
| 1:A1:408:ARG:HH12 | 11:K1:15:ARG:HE    | 1.22                     | 0.84              |
| 5:Q1:134:ILE:HD11 | 5:Q1:185:TYR:CG    | 2.12                     | 0.84              |
| 2:B1:213:HIS:N    | 2:B1:214:PRO:HD2   | 1.91                     | 0.84              |
| 10:J1:21:ALA:O    | 10:J1:25:VAL:HG23  | 1.77                     | 0.84              |
| 1:M1:32:GLN:CG    | 1:M1:33:PRO:HD2    | 2.08                     | 0.84              |
| 2:N1:58:GLU:OE1   | 2:N1:63:LEU:HA     | 1.77                     | 0.84              |
| 2:N1:126:VAL:O    | 2:N1:130:PRO:HG3   | 1.78                     | 0.84              |
| 1:A1:61:HIS:NE2   | 1:A1:134:ILE:HD11  | 1.91                     | 0.84              |
| 1:A1:84:ALA:HB2   | 1:A1:101:ALA:HB2   | 1.59                     | 0.84              |
| 1:M1:378:ASP:O    | 1:M1:382:SER:HB2   | 1.77                     | 0.84              |
| 3:O1:245:PHE:CD1  | 4:P1:17:LEU:HD13   | 2.11                     | 0.84              |
| 2:B1:57:TYR:O     | 2:B1:233:SER:HB2   | 1.77                     | 0.84              |
| 2:B1:263:ALA:O    | 2:B1:269:ALA:HB2   | 1.76                     | 0.84              |
| 3:C1:115:ILE:CG2  | 3:C1:196:HIS:HB2   | 2.08                     | 0.84              |
| 7:G1:73:ASN:N     | 7:G1:74:PRO:HD2    | 1.91                     | 0.84              |
| 10:J1:18:SER:OG   | 11:K1:23:LEU:HB2   | 1.78                     | 0.84              |
| 2:B1:198:HIS:HE1  | 2:B1:233:SER:HB3   | 1.42                     | 0.84              |
| 1:M1:67:THR:HG23  | 1:M1:70:ARG:N      | 1.92                     | 0.84              |
| 19:A2:159:ALA:HB3 | 27:I2:84:VAL:CG1   | 2.08                     | 0.84              |
| 1:A1:106:LEU:HD22 | 1:A1:203:LEU:HD22  | 1.60                     | 0.84              |
| 6:F1:51:PRO:HD3   | 2:N1:134:ARG:NH1   | 1.93                     | 0.84              |
| 1:A1:308:GLN:O    | 1:A1:308:GLN:HG3   | 1.77                     | 0.83              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C1:163:TRP:CZ2  | 5:Q1:62:MET:HE2    | 2.13                     | 0.83              |
| 1:M1:40:TRP:CZ2   | 1:M1:377:GLU:HA    | 2.13                     | 0.83              |
| 6:R1:37:ILE:HG12  | 6:R1:43:VAL:HG21   | 1.59                     | 0.83              |
| 57:B3:78:LEU:HB2  | 57:B3:79:PRO:HD3   | 1.58                     | 0.83              |
| 2:N1:341:TYR:HE2  | 2:N1:345:LYS:HE3   | 1.41                     | 0.83              |
| 5:Q1:114:VAL:HA   | 5:Q1:117:LEU:CD1   | 2.06                     | 0.83              |
| 56:A3:187:SER:HB2 | 56:A3:277:MET:HE1  | 1.60                     | 0.83              |
| 1:A1:39:VAL:HG12  | 1:A1:41:ILE:HD11   | 1.59                     | 0.83              |
| 3:C1:47:THR:HG21  | 3:C1:83:HIS:HB2    | 1.61                     | 0.83              |
| 1:M1:106:LEU:HD22 | 1:M1:203:LEU:HD22  | 1.59                     | 0.83              |
| 4:D1:17:LEU:O     | 4:D1:202:LYS:HD3   | 1.78                     | 0.83              |
| 4:D1:70:VAL:HG23  | 4:D1:84:PRO:HD3    | 1.59                     | 0.83              |
| 1:A1:426:GLY:HA3  | 1:A1:428:ILE:HG13  | 1.59                     | 0.83              |
| 3:C1:213:SER:O    | 3:C1:216:ASP:N     | 2.10                     | 0.83              |
| 1:M1:383:LEU:HA   | 1:M1:387:GLY:O     | 1.78                     | 0.83              |
| 17:82:424:ILE:CG1 | 19:A2:76:ARG:HH21  | 1.92                     | 0.83              |
| 2:N1:56:ARG:NH2   | 2:N1:318:ASP:OD1   | 2.12                     | 0.82              |
| 19:A2:312:GLY:N   | 38:U2:142:THR:O    | 2.12                     | 0.82              |
| 5:Q1:76:ILE:HG23  | 5:Q1:194:ILE:HG12  | 1.60                     | 0.82              |
| 1:A1:408:ARG:HH22 | 11:K1:15:ARG:CZ    | 1.90                     | 0.82              |
| 4:D1:178:THR:HB   | 4:D1:181:GLN:HG3   | 1.60                     | 0.82              |
| 6:F1:6:VAL:HB     | 6:F1:10:SER:HB2    | 1.60                     | 0.82              |
| 1:M1:428:ILE:CG2  | 1:M1:431:LEU:HD22  | 2.07                     | 0.82              |
| 1:A1:145:MET:SD   | 1:A1:248:LEU:HD12  | 2.18                     | 0.82              |
| 1:M1:408:ARG:HH22 | 11:W1:15:ARG:CZ    | 1.91                     | 0.82              |
| 2:N1:217:LYS:HZ2  | 2:N1:221:GLU:CD    | 1.87                     | 0.82              |
| 19:A2:613:PRO:HB2 | 38:U2:134:ILE:HD13 | 1.60                     | 0.82              |
| 1:A1:241:ILE:HG13 | 7:G1:16:TYR:CE1    | 2.15                     | 0.82              |
| 7:G1:30:PHE:O     | 7:G1:34:ILE:HG13   | 1.78                     | 0.82              |
| 4:P1:41:HIS:CD2   | 4:P1:113:LEU:HD11  | 2.15                     | 0.82              |
| 4:P1:176:PRO:HB2  | 4:P1:181:GLN:HE22  | 1.44                     | 0.82              |
| 7:S1:72:LYS:CB    | 7:S1:75:ALA:HB2    | 2.09                     | 0.82              |
| 3:C1:119:LEU:HG   | 69:C1:402:HEM:CBB  | 2.09                     | 0.82              |
| 4:D1:50:HIS:HB3   | 4:D1:54:VAL:HB     | 1.62                     | 0.82              |
| 7:G1:50:PRO:HB2   | 7:G1:51:PRO:HD3    | 1.61                     | 0.82              |
| 19:A2:302:LEU:HA  | 38:U2:137:TRP:HB2  | 1.59                     | 0.82              |
| 3:O1:297:SER:O    | 3:O1:300:ILE:HG22  | 1.79                     | 0.82              |
| 7:S1:50:PRO:CB    | 7:S1:51:PRO:HD3    | 2.09                     | 0.82              |
| 3:O1:234:LEU:CD2  | 4:P1:216:LEU:HD21  | 2.08                     | 0.82              |
| 19:A2:128:CYS:SG  | 75:A2:801:SF4:S1   | 2.78                     | 0.81              |
| 2:B1:198:HIS:CE1  | 2:B1:233:SER:HB3   | 2.14                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O1:26:ASN:HD21  | 3:O1:207:ASN:CB   | 1.90                     | 0.81              |
| 1:A1:18:GLN:NE2   | 1:A1:22:GLY:HA2   | 1.94                     | 0.81              |
| 1:A1:408:ARG:NH2  | 11:K1:15:ARG:NE   | 2.28                     | 0.81              |
| 3:C1:27:ILE:O     | 3:C1:27:ILE:HG22  | 1.79                     | 0.81              |
| 4:D1:220:TYR:CE2  | 7:G1:26:PHE:HE1   | 1.97                     | 0.81              |
| 2:N1:279:LEU:HB3  | 2:N1:295:LEU:HD22 | 1.60                     | 0.81              |
| 2:N1:331:ALA:HA   | 2:N1:432:HIS:ND1  | 1.96                     | 0.81              |
| 4:P1:10:TYR:HE1   | 8:T1:73:LEU:HD21  | 1.46                     | 0.81              |
| 1:A1:379:ILE:HD12 | 1:A1:390:ILE:HD12 | 1.62                     | 0.81              |
| 1:A1:53:ASN:OD1   | 1:A1:165:GLN:HB2  | 1.80                     | 0.81              |
| 2:B1:169:ARG:NH2  | 2:N1:438:GLU:OE2  | 2.14                     | 0.81              |
| 3:O1:218:ILE:CG2  | 3:O1:223:TYR:CD2  | 2.63                     | 0.81              |
| 19:A2:425:ASN:O   | 25:G2:169:ARG:NH1 | 2.13                     | 0.81              |
| 3:C1:341:GLN:HB3  | 3:C1:347:TYR:CD2  | 2.15                     | 0.81              |
| 8:H1:21:ARG:HB3   | 8:H1:65:ARG:HH21  | 1.45                     | 0.81              |
| 2:B1:42:ALA:HB1   | 2:B1:43:PRO:HD2   | 1.62                     | 0.81              |
| 5:Q1:99:ARG:HD3   | 5:Q1:156:TYR:OH   | 1.80                     | 0.81              |
| 44:a2:79:ASN:ND2  | 55:e2:76:PRO:HD3  | 1.96                     | 0.81              |
| 1:A1:102:LEU:HB2  | 1:A1:105:ASP:OD2  | 1.81                     | 0.81              |
| 3:C1:266:PRO:HA   | 5:Q1:160:CYS:SG   | 2.21                     | 0.81              |
| 52:12:75:PRO:N    | 52:12:223:PHE:HZ  | 1.79                     | 0.81              |
| 62:G3:5:LYS:NZ    | 62:G3:6:GLY:H     | 1.78                     | 0.81              |
| 1:A1:426:GLY:CA   | 1:A1:428:ILE:CG1  | 2.59                     | 0.81              |
| 2:B1:248:ASN:HB2  | 2:B1:428:GLY:HA2  | 1.63                     | 0.80              |
| 9:I1:78:TYR:OXT   | 9:I1:78:TYR:HD1   | 1.63                     | 0.80              |
| 1:M1:67:THR:HG22  | 1:M1:70:ARG:HB2   | 1.61                     | 0.80              |
| 3:O1:106:SER:O    | 3:O1:109:PHE:HD2  | 1.63                     | 0.80              |
| 2:B1:185:LYS:HG3  | 2:B1:185:LYS:O    | 1.79                     | 0.80              |
| 2:B1:394:PRO:O    | 2:B1:398:VAL:HG23 | 1.80                     | 0.80              |
| 3:C1:33:PHE:CE1   | 3:C1:96:MET:HG3   | 2.16                     | 0.80              |
| 5:E1:15:ARG:CB    | 5:E1:16:PRO:HD2   | 2.08                     | 0.80              |
| 8:T1:50:THR:HG22  | 8:T1:52:GLU:H     | 1.47                     | 0.80              |
| 17:82:424:ILE:CG1 | 19:A2:76:ARG:NH2  | 2.44                     | 0.80              |
| 5:Q1:118:ARG:NH1  | 5:Q1:171:ILE:HG13 | 1.95                     | 0.80              |
| 10:V1:58:LYS:HG2  | 10:V1:59:TYR:N    | 1.97                     | 0.80              |
| 63:H3:39:CYS:SG   | 63:H3:53:CYS:HB3  | 2.22                     | 0.80              |
| 1:A1:42:ASP:HB3   | 1:A1:384:LEU:HD22 | 1.62                     | 0.80              |
| 5:E1:31:ALA:HB2   | 10:J1:7:ALA:HB2   | 1.63                     | 0.80              |
| 1:M1:182:LEU:O    | 1:M1:186:LEU:HD12 | 1.82                     | 0.80              |
| 1:M1:445:ARG:O    | 1:M1:446:PHE:HB2  | 1.79                     | 0.80              |
| 2:N1:200:THR:CG2  | 2:N1:203:ARG:HD2  | 2.10                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:126:THR:OG1   | 3:O1:185:LEU:HD23  | 1.82                     | 0.80              |
| 4:P1:10:TYR:HE1    | 8:T1:73:LEU:CD2    | 1.94                     | 0.80              |
| 4:P1:220:TYR:CE2   | 7:S1:26:PHE:HE1    | 1.98                     | 0.80              |
| 3:C1:51:LEU:HD11   | 3:C1:80:ARG:HA     | 1.63                     | 0.80              |
| 69:O1:401:HEM:HBC2 | 69:O1:401:HEM:HMC1 | 1.61                     | 0.80              |
| 6:R1:33:ARG:NH2    | 6:R1:91:GLU:OE2    | 2.14                     | 0.80              |
| 2:B1:305:GLN:HB2   | 2:B1:306:PRO:CD    | 2.11                     | 0.80              |
| 3:C1:5:ARG:O       | 3:C1:9:PRO:HD2     | 1.82                     | 0.80              |
| 7:G1:72:LYS:CB     | 7:G1:75:ALA:HB2    | 2.09                     | 0.80              |
| 8:T1:21:ARG:HB3    | 8:T1:65:ARG:NH2    | 1.95                     | 0.80              |
| 2:B1:207:ILE:HD11  | 2:B1:383:GLY:HA2   | 1.62                     | 0.80              |
| 5:E1:41:ALA:O      | 5:E1:45:VAL:HG23   | 1.81                     | 0.80              |
| 1:A1:426:GLY:N     | 1:A1:428:ILE:CG1   | 2.45                     | 0.80              |
| 3:C1:3:ASN:N       | 3:C1:8:HIS:NE2     | 2.30                     | 0.80              |
| 2:N1:24:LEU:H      | 2:N1:24:LEU:HD12   | 1.47                     | 0.80              |
| 3:C1:218:ILE:CG2   | 3:C1:223:TYR:CD2   | 2.65                     | 0.79              |
| 2:B1:168:TYR:HB2   | 2:B1:173:ALA:HB2   | 1.63                     | 0.79              |
| 3:O1:185:LEU:HB3   | 3:O1:186:PRO:HD3   | 1.61                     | 0.79              |
| 52:12:126:LYS:O    | 52:12:129:LEU:N    | 2.15                     | 0.79              |
| 2:B1:209:LEU:HD22  | 2:B1:375:SER:HB2   | 1.64                     | 0.79              |
| 3:C1:169:SER:HB2   | 5:Q1:93:GLY:HA3    | 1.64                     | 0.79              |
| 4:D1:220:TYR:HE2   | 7:G1:26:PHE:HE1    | 1.30                     | 0.79              |
| 1:M1:260:PRO:HD3   | 1:M1:414:TYR:CE1   | 2.18                     | 0.79              |
| 4:P1:27:ARG:HH12   | 10:V1:58:LYS:HG3   | 1.46                     | 0.79              |
| 1:A1:428:ILE:HG22  | 1:A1:431:LEU:CB    | 2.12                     | 0.79              |
| 2:B1:362:ASN:HA    | 2:B1:365:LYS:HD3   | 1.65                     | 0.79              |
| 10:J1:58:LYS:HG2   | 10:J1:59:TYR:N     | 1.96                     | 0.79              |
| 2:N1:68:LEU:HD23   | 2:N1:186:VAL:CG1   | 2.12                     | 0.79              |
| 3:O1:102:LEU:HD21  | 3:O1:304:ILE:CD1   | 2.12                     | 0.79              |
| 6:R1:51:PRO:HG2    | 6:R1:54:LEU:CD2    | 2.12                     | 0.79              |
| 1:A1:155:ALA:HA    | 1:A1:164:ALA:HB1   | 1.63                     | 0.79              |
| 3:O1:135:TRP:CH2   | 3:O1:170:VAL:HG12  | 2.17                     | 0.79              |
| 5:Q1:91:TRP:HB3    | 5:Q1:96:LEU:HB2    | 1.62                     | 0.79              |
| 1:M1:408:ARG:NH2   | 11:W1:15:ARG:NE    | 2.30                     | 0.79              |
| 2:N1:261:SER:OG    | 2:N1:320:GLY:HA3   | 1.83                     | 0.79              |
| 4:P1:138:PRO:HG2   | 8:T1:55:THR:OG1    | 1.82                     | 0.79              |
| 8:T1:73:LEU:HD23   | 8:T1:74:PHE:N      | 1.98                     | 0.79              |
| 3:C1:111:GLU:O     | 3:C1:115:ILE:HD13  | 1.82                     | 0.79              |
| 3:C1:264:THR:HG21  | 5:Q1:144:CYS:CB    | 2.13                     | 0.79              |
| 2:N1:159:VAL:HG12  | 2:N1:160:ILE:HD13  | 1.65                     | 0.79              |
| 3:O1:246:ALA:HB1   | 3:O1:249:LEU:HB2   | 1.65                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:86:LEU:HD13   | 1:A1:99:ILE:HG12   | 1.64                     | 0.79              |
| 3:O1:316:MET:HE2   | 3:O1:317:PHE:CE1   | 2.17                     | 0.79              |
| 63:H3:39:CYS:SG    | 63:H3:53:CYS:CB    | 2.70                     | 0.79              |
| 4:D1:10:TYR:CZ     | 4:D1:128:PHE:HE2   | 2.01                     | 0.79              |
| 5:Q1:114:VAL:CA    | 5:Q1:117:LEU:HD12  | 2.12                     | 0.79              |
| 10:V1:58:LYS:HG2   | 10:V1:59:TYR:H     | 1.48                     | 0.79              |
| 19:A2:674:LEU:HD12 | 29:K2:46:LYS:CE    | 2.13                     | 0.79              |
| 3:C1:280:ILE:HD11  | 3:C1:335:LEU:HD13  | 1.64                     | 0.78              |
| 1:M1:39:VAL:HG12   | 1:M1:41:ILE:HD11   | 1.65                     | 0.78              |
| 10:V1:3:PRO:HG2    | 10:V1:8:ARG:HG2    | 1.63                     | 0.78              |
| 19:A2:426:ASP:HA   | 25:G2:169:ARG:HH12 | 1.48                     | 0.78              |
| 1:M1:262:TRP:CD2   | 1:M1:385:THR:HG23  | 2.18                     | 0.78              |
| 2:B1:297:GLN:OE1   | 2:B1:297:GLN:HA    | 1.82                     | 0.78              |
| 2:B1:304:HIS:HD2   | 2:B1:306:PRO:HD2   | 1.48                     | 0.78              |
| 2:B1:385:GLN:CG    | 9:I1:62:ARG:HH12   | 1.96                     | 0.78              |
| 4:P1:198:HIS:NE2   | 4:P1:202:LYS:NZ    | 2.31                     | 0.78              |
| 4:P1:220:TYR:HE2   | 7:S1:26:PHE:HE1    | 1.29                     | 0.78              |
| 19:A2:302:LEU:HA   | 38:U2:137:TRP:HB3  | 1.64                     | 0.78              |
| 19:A2:302:LEU:CA   | 38:U2:137:TRP:CB   | 2.60                     | 0.78              |
| 4:D1:74:PRO:CB     | 4:D1:79:GLU:HB2    | 2.13                     | 0.78              |
| 7:G1:44:CYS:SG     | 7:G1:48:VAL:HG21   | 2.22                     | 0.78              |
| 2:N1:309:VAL:HG22  | 2:N1:326:THR:HA    | 1.63                     | 0.78              |
| 36:S2:200:PRO:CG   | 36:S2:223:GLN:HE22 | 1.93                     | 0.78              |
| 63:H3:75:ARG:HG2   | 63:H3:75:ARG:HH11  | 1.48                     | 0.78              |
| 3:C1:51:LEU:HD21   | 3:C1:79:ILE:HG22   | 1.63                     | 0.78              |
| 3:C1:275:LEU:O     | 3:C1:276:PHE:C     | 2.23                     | 0.78              |
| 4:D1:3:LEU:HD11    | 7:G1:71:ARG:HB2    | 1.64                     | 0.78              |
| 4:P1:115:TYR:HD1   | 4:P1:119:ALA:HB2   | 1.47                     | 0.78              |
| 9:U1:64:LEU:HG     | 9:U1:65:VAL:HG23   | 1.65                     | 0.78              |
| 47:d2:25:PHE:HD2   | 47:d2:40:VAL:CB    | 1.93                     | 0.78              |
| 2:B1:438:GLU:OE2   | 2:N1:169:ARG:NH2   | 2.16                     | 0.78              |
| 3:O1:1:MET:SD      | 3:O1:7:SER:HB2     | 2.23                     | 0.78              |
| 4:D1:228:SER:HB2   | 7:G1:23:GLN:NE2    | 1.98                     | 0.78              |
| 7:G1:31:SER:O      | 7:G1:35:PRO:HD2    | 1.83                     | 0.78              |
| 1:M1:297:ILE:HG22  | 1:M1:303:LEU:HD12  | 1.63                     | 0.78              |
| 2:B1:347:ILE:O     | 2:B1:411:ILE:HG23  | 1.83                     | 0.78              |
| 4:P1:10:TYR:CZ     | 4:P1:128:PHE:HE2   | 2.01                     | 0.78              |
| 1:A1:45:SER:HB3    | 1:A1:92:ARG:HA     | 1.66                     | 0.78              |
| 2:N1:308:ASP:OD1   | 2:N1:309:VAL:N     | 2.17                     | 0.78              |
| 3:O1:309:THR:CG2   | 3:O1:370:GLY:HA3   | 2.14                     | 0.78              |
| 19:A2:557:ARG:HH21 | 38:U2:144:TYR:HH   | 1.30                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:D2:107:ASP:OD2 | 22:D2:113:PHE:CE1  | 2.37                     | 0.77              |
| 2:N1:286:LYS:HD3  | 2:N1:287:ARG:NH1   | 1.98                     | 0.77              |
| 1:M1:32:GLN:HG3   | 1:M1:33:PRO:HD2    | 1.66                     | 0.77              |
| 5:Q1:65:SER:OG    | 5:Q1:67:ASP:HB3    | 1.85                     | 0.77              |
| 2:N1:297:GLN:OE1  | 2:N1:297:GLN:HA    | 1.83                     | 0.77              |
| 3:C1:106:SER:O    | 3:C1:109:PHE:HD1   | 1.66                     | 0.77              |
| 3:C1:108:THR:HB   | 3:C1:313:ARG:NH1   | 2.00                     | 0.77              |
| 4:D1:14:HIS:HA    | 4:D1:19:SER:HB3    | 1.66                     | 0.77              |
| 2:N1:341:TYR:CE2  | 2:N1:345:LYS:HE3   | 2.19                     | 0.77              |
| 1:A1:46:ARG:NH2   | 1:A1:316:ASP:OD2   | 2.17                     | 0.77              |
| 3:O1:341:GLN:HB3  | 3:O1:347:TYR:CD2   | 2.19                     | 0.77              |
| 7:S1:9:ARG:HH21   | 7:S1:11:ARG:HD2    | 1.44                     | 0.77              |
| 1:A1:39:VAL:HG12  | 1:A1:41:ILE:CD1    | 2.13                     | 0.77              |
| 2:B1:331:ALA:HA   | 2:B1:432:HIS:ND1   | 2.00                     | 0.77              |
| 3:C1:26:ASN:ND2   | 3:C1:207:ASN:HB2   | 1.99                     | 0.77              |
| 1:M1:21:ASN:HB3   | 1:M1:217:SER:CB    | 2.13                     | 0.77              |
| 1:M1:75:LEU:O     | 1:M1:79:VAL:HG23   | 1.82                     | 0.77              |
| 4:P1:50:HIS:HB3   | 4:P1:54:VAL:HB     | 1.64                     | 0.77              |
| 1:A1:386:TYR:HD1  | 1:A1:386:TYR:H     | 1.32                     | 0.77              |
| 1:M1:92:ARG:HD2   | 1:M1:163:LEU:HD12  | 1.65                     | 0.77              |
| 3:O1:170:VAL:HG13 | 3:O1:174:THR:HG21  | 1.66                     | 0.77              |
| 6:F1:28:LYS:CD    | 6:F1:74:ILE:HD11   | 2.14                     | 0.77              |
| 19:A2:159:ALA:HB3 | 27:I2:84:VAL:HG11  | 1.65                     | 0.77              |
| 20:B2:94:VAL:CG1  | 20:B2:115:LEU:HD22 | 2.12                     | 0.77              |
| 1:A1:21:ASN:HB3   | 1:A1:217:SER:OG    | 1.84                     | 0.76              |
| 3:C1:310:SER:HB3  | 3:C1:318:ARG:HH11  | 1.47                     | 0.76              |
| 3:C1:338:ILE:HD12 | 3:C1:338:ILE:N     | 1.99                     | 0.76              |
| 4:D1:182:VAL:O    | 4:D1:186:VAL:HG23  | 1.84                     | 0.76              |
| 1:M1:331:ILE:HD11 | 1:M1:427:PRO:O     | 1.85                     | 0.76              |
| 3:O1:310:SER:OG   | 3:O1:318:ARG:NH1   | 2.18                     | 0.76              |
| 2:B1:101:THR:HG23 | 2:B1:104:ASN:H     | 1.48                     | 0.76              |
| 4:P1:143:LEU:HD22 | 4:P1:147:LEU:O     | 1.86                     | 0.76              |
| 5:Q1:157:TYR:OH   | 5:Q1:162:GLY:HA2   | 1.84                     | 0.76              |
| 57:B3:5:MET:HE3   | 66:K3:42:PRO:HA    | 1.67                     | 0.76              |
| 2:B1:59:ASN:O     | 2:B1:63:LEU:HG     | 1.84                     | 0.76              |
| 2:N1:29:LEU:HB3   | 2:N1:30:PRO:CD     | 2.14                     | 0.76              |
| 3:C1:187:PHE:CZ   | 3:O1:184:ILE:HG13  | 2.20                     | 0.76              |
| 4:D1:229:VAL:HG12 | 4:D1:233:ARG:HE    | 1.49                     | 0.76              |
| 3:O1:206:ASN:CB   | 3:O1:313:ARG:HH21  | 1.99                     | 0.76              |
| 4:P1:55:CYS:SG    | 10:V1:52:TRP:HB2   | 2.25                     | 0.76              |
| 4:P1:178:THR:OG1  | 4:P1:181:GLN:NE2   | 2.14                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:Q1:153:PHE:HE1   | 5:Q1:173:LYS:HG3  | 1.50                     | 0.76              |
| 27:I2:104:ASP:O    | 27:I2:105:LYS:CB  | 2.30                     | 0.76              |
| 2:B1:67:HIS:CD2    | 2:B1:144:LEU:HD22 | 2.18                     | 0.76              |
| 2:B1:148:LYS:HE2   | 2:B1:180:ASP:OD1  | 1.85                     | 0.76              |
| 1:M1:24:ARG:CB     | 1:M1:196:VAL:HG22 | 2.14                     | 0.76              |
| 2:N1:200:THR:HG22  | 2:N1:203:ARG:CD   | 2.15                     | 0.76              |
| 6:R1:73:GLN:NE2    | 7:S1:32:LYS:NZ    | 2.33                     | 0.76              |
| 1:A1:92:ARG:HD2    | 1:A1:163:LEU:HD12 | 1.67                     | 0.76              |
| 1:A1:146:ARG:NH2   | 1:A1:308:GLN:HE22 | 1.82                     | 0.76              |
| 3:C1:210:GLY:HA3   | 3:C1:314:SER:HB2  | 1.68                     | 0.76              |
| 3:O1:3:ASN:N       | 3:O1:8:HIS:NE2    | 2.32                     | 0.76              |
| 4:P1:181:GLN:HA    | 8:T1:77:LEU:HD13  | 1.67                     | 0.76              |
| 18:92:42:ARG:HH12  | 19:A2:199:GLY:CA  | 1.96                     | 0.76              |
| 3:C1:9:PRO:HG2     | 3:C1:12:LYS:HB2   | 1.68                     | 0.76              |
| 2:N1:213:HIS:N     | 2:N1:214:PRO:HD2  | 2.01                     | 0.76              |
| 2:N1:305:GLN:CB    | 2:N1:306:PRO:HD3  | 2.15                     | 0.76              |
| 1:A1:27:SER:HA     | 1:A1:199:ALA:O    | 1.86                     | 0.76              |
| 3:C1:47:THR:CG2    | 3:C1:83:HIS:HB2   | 2.16                     | 0.76              |
| 6:F1:94:LEU:O      | 6:F1:98:ILE:HG13  | 1.86                     | 0.76              |
| 1:M1:41:ILE:H      | 1:M1:41:ILE:HD12  | 1.50                     | 0.76              |
| 19:A2:313:LEU:CA   | 38:U2:142:THR:HA  | 2.15                     | 0.76              |
| 1:M1:102:LEU:HB2   | 1:M1:105:ASP:OD2  | 1.85                     | 0.75              |
| 2:N1:257:LEU:HD13  | 2:N1:424:MET:HB2  | 1.68                     | 0.75              |
| 19:A2:313:LEU:HD23 | 38:U2:142:THR:CA  | 2.16                     | 0.75              |
| 5:E1:55:VAL:O      | 5:E1:59:VAL:HG23  | 1.85                     | 0.75              |
| 6:R1:28:LYS:CD     | 6:R1:74:ILE:HD11  | 2.15                     | 0.75              |
| 19:A2:312:GLY:N    | 38:U2:143:PRO:C   | 2.45                     | 0.75              |
| 19:A2:314:LEU:HD23 | 38:U2:140:PRO:CD  | 2.04                     | 0.75              |
| 2:B1:141:GLN:HB2   | 2:B1:142:PRO:HD3  | 1.68                     | 0.75              |
| 4:D1:127:VAL:HG12  | 4:D1:187:CYS:SG   | 2.26                     | 0.75              |
| 57:B3:59:GLN:H     | 57:B3:62:GLU:HG3  | 1.51                     | 0.75              |
| 1:A1:249:PRO:O     | 1:A1:250:LEU:HD23 | 1.85                     | 0.75              |
| 3:C1:310:SER:CB    | 3:C1:318:ARG:HH11 | 1.99                     | 0.75              |
| 3:O1:47:THR:CG2    | 3:O1:83:HIS:HB2   | 2.16                     | 0.75              |
| 3:O1:129:MET:HG2   | 3:O1:178:PHE:HD1  | 1.49                     | 0.75              |
| 10:J1:51:LEU:HD22  | 10:J1:52:TRP:HZ3  | 1.50                     | 0.75              |
| 9:U1:72:VAL:CB     | 9:U1:73:PRO:HD3   | 2.15                     | 0.75              |
| 52:12:75:PRO:CA    | 52:12:223:PHE:CE1 | 2.69                     | 0.75              |
| 2:B1:207:ILE:HD12  | 2:B1:382:VAL:HG12 | 1.69                     | 0.75              |
| 2:N1:314:ALA:CB    | 9:U1:64:LEU:HD22  | 2.17                     | 0.75              |
| 3:O1:61:THR:O      | 3:O1:62:ALA:C     | 2.30                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:177:ARG:O     | 3:O1:181:PHE:HD2   | 1.69                     | 0.75              |
| 5:Q1:134:ILE:HD11  | 5:Q1:185:TYR:CE2   | 2.22                     | 0.75              |
| 5:Q1:171:ILE:CD1   | 5:Q1:176:ALA:HB3   | 2.17                     | 0.75              |
| 6:R1:50:LEU:HB2    | 6:R1:55:TYR:HB2    | 1.67                     | 0.75              |
| 1:A1:145:MET:HE3   | 1:A1:252:HIS:CE1   | 2.21                     | 0.75              |
| 2:N1:59:ASN:O      | 2:N1:63:LEU:HG     | 1.87                     | 0.75              |
| 3:O1:310:SER:CB    | 3:O1:318:ARG:HH11  | 2.00                     | 0.75              |
| 5:Q1:77:LYS:HG3    | 5:Q1:89:PHE:CE2    | 2.22                     | 0.75              |
| 7:G1:9:ARG:HH21    | 7:G1:11:ARG:HD2    | 1.49                     | 0.75              |
| 2:N1:49:LEU:HD11   | 2:N1:204:MET:SD    | 2.26                     | 0.75              |
| 19:A2:613:PRO:HB2  | 38:U2:134:ILE:CD1  | 2.17                     | 0.75              |
| 1:A1:236:PHE:HD2   | 1:A1:258:GLU:HG2   | 1.52                     | 0.75              |
| 1:M1:386:TYR:HD1   | 1:M1:386:TYR:H     | 1.33                     | 0.75              |
| 58:C3:187:THR:HG21 | 62:G3:68:THR:HG21  | 1.68                     | 0.75              |
| 3:C1:169:SER:OG    | 3:C1:170:VAL:N     | 2.18                     | 0.74              |
| 3:C1:345:HIS:HB3   | 3:C1:346:PRO:CD    | 2.17                     | 0.74              |
| 3:C1:361:LEU:HD23  | 3:C1:365:LEU:HD12  | 1.69                     | 0.74              |
| 5:Q1:118:ARG:HH11  | 5:Q1:171:ILE:HG13  | 1.50                     | 0.74              |
| 19:A2:181:ARG:HB3  | 75:A2:802:SF4:S2   | 2.27                     | 0.74              |
| 19:A2:426:ASP:CA   | 25:G2:169:ARG:HH12 | 1.98                     | 0.74              |
| 1:A1:72:GLY:O      | 1:A1:73:ASN:OD1    | 2.04                     | 0.74              |
| 3:C1:126:THR:OG1   | 3:C1:185:LEU:HD23  | 1.87                     | 0.74              |
| 2:N1:304:HIS:HD2   | 2:N1:306:PRO:HD2   | 1.51                     | 0.74              |
| 1:A1:316:ASP:OD1   | 1:A1:316:ASP:N     | 2.21                     | 0.74              |
| 4:D1:5:LEU:HB3     | 4:D1:152:TYR:CD1   | 2.22                     | 0.74              |
| 1:M1:39:VAL:HG23   | 1:M1:113:LEU:HD23  | 1.68                     | 0.74              |
| 3:O1:90:PHE:CE1    | 3:O1:123:VAL:HG21  | 2.22                     | 0.74              |
| 1:M1:18:GLN:NE2    | 1:M1:22:GLY:HA2    | 2.01                     | 0.74              |
| 5:Q1:118:ARG:HD2   | 5:Q1:171:ILE:HG12  | 1.70                     | 0.74              |
| 18:92:42:ARG:NH2   | 19:A2:199:GLY:HA3  | 2.03                     | 0.74              |
| 22:D2:107:ASP:OD2  | 22:D2:113:PHE:HE1  | 1.70                     | 0.74              |
| 3:C1:206:ASN:ND2   | 3:C1:207:ASN:H     | 1.85                     | 0.74              |
| 19:A2:426:ASP:HA   | 25:G2:169:ARG:NH1  | 2.03                     | 0.74              |
| 1:A1:84:ALA:CB     | 1:A1:101:ALA:HB2   | 2.18                     | 0.74              |
| 3:C1:7:SER:HA      | 3:C1:13:ILE:HG12   | 1.69                     | 0.74              |
| 4:D1:11:PRO:O      | 8:H1:74:PHE:CE2    | 2.41                     | 0.74              |
| 1:M1:53:ASN:OD1    | 1:M1:165:GLN:HB2   | 1.87                     | 0.74              |
| 1:M1:99:ILE:HG13   | 1:M1:113:LEU:HD13  | 1.69                     | 0.74              |
| 2:N1:68:LEU:HD23   | 2:N1:186:VAL:HG12  | 1.69                     | 0.74              |
| 19:A2:144:MET:HG2  | 20:B2:380:HIS:CD2  | 2.23                     | 0.74              |
| 1:A1:75:LEU:O      | 1:A1:79:VAL:HG23   | 1.88                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:292:SER:O     | 1:A1:295:ALA:HB3   | 1.88                     | 0.74              |
| 2:B1:337:ILE:HG21  | 2:B1:434:PRO:HG2   | 1.68                     | 0.74              |
| 19:A2:161:GLU:CB   | 27:I2:102:ASN:ND2  | 2.50                     | 0.74              |
| 52:12:17:VAL:HG23  | 52:12:225:MET:HE1  | 1.68                     | 0.74              |
| 1:A1:236:PHE:CD2   | 1:A1:258:GLU:HG2   | 2.22                     | 0.74              |
| 1:A1:334:MET:HA    | 1:A1:334:MET:HE3   | 1.70                     | 0.74              |
| 2:B1:140:LEU:O     | 2:B1:141:GLN:C     | 2.30                     | 0.74              |
| 3:C1:184:ILE:HG13  | 3:O1:187:PHE:CZ    | 2.23                     | 0.74              |
| 1:A1:408:ARG:CZ    | 11:K1:15:ARG:HE    | 2.01                     | 0.73              |
| 8:H1:15:ASP:N      | 8:H1:16:PRO:HD2    | 2.03                     | 0.73              |
| 2:N1:237:ALA:HB2   | 2:N1:318:ASP:OD2   | 1.87                     | 0.73              |
| 5:Q1:188:THR:N     | 5:Q1:192:MET:O     | 2.21                     | 0.73              |
| 2:B1:162:ASN:HD22  | 2:B1:244:ILE:HG21  | 1.51                     | 0.73              |
| 3:O1:122:THR:CG2   | 3:O1:189:ILE:HD11  | 2.17                     | 0.73              |
| 3:O1:184:ILE:O     | 3:O1:188:ILE:HD12  | 1.88                     | 0.73              |
| 5:Q1:121:GLN:O     | 5:Q1:170:ARG:NH1   | 2.18                     | 0.73              |
| 57:B3:184:LEU:HD11 | 57:B3:211:LEU:HD21 | 1.69                     | 0.73              |
| 1:A1:236:PHE:HE2   | 1:A1:258:GLU:HB3   | 1.50                     | 0.73              |
| 1:A1:383:LEU:HA    | 1:A1:387:GLY:O     | 1.88                     | 0.73              |
| 2:B1:129:ALA:N     | 2:B1:130:PRO:HD2   | 2.01                     | 0.73              |
| 1:M1:408:ARG:HH12  | 11:W1:15:ARG:NE    | 1.85                     | 0.73              |
| 5:Q1:55:VAL:O      | 5:Q1:59:VAL:HG23   | 1.88                     | 0.73              |
| 5:Q1:157:TYR:HE2   | 5:Q1:159:PRO:HA    | 1.51                     | 0.73              |
| 2:B1:78:LYS:HB3    | 2:B1:129:ALA:HB1   | 1.70                     | 0.73              |
| 2:B1:347:ILE:H     | 2:B1:347:ILE:HD12  | 1.54                     | 0.73              |
| 1:M1:426:GLY:CA    | 1:M1:428:ILE:CG1   | 2.64                     | 0.73              |
| 2:N1:385:GLN:CG    | 9:U1:62:ARG:HH12   | 2.00                     | 0.73              |
| 3:C1:280:ILE:CD1   | 3:C1:335:LEU:HD13  | 2.19                     | 0.73              |
| 1:M1:256:ALA:HA    | 1:M1:320:LEU:O     | 1.89                     | 0.73              |
| 1:M1:363:ASN:OD1   | 2:N1:112:LEU:HD23  | 1.88                     | 0.73              |
| 2:N1:34:VAL:HG11   | 2:N1:386:ALA:HB1   | 1.70                     | 0.73              |
| 2:N1:95:LYS:HE3    | 9:U1:70:LEU:HD22   | 1.69                     | 0.73              |
| 3:O1:361:LEU:CD2   | 3:O1:365:LEU:HD12  | 2.18                     | 0.73              |
| 17:82:424:ILE:HD11 | 19:A2:76:ARG:HH21  | 1.51                     | 0.73              |
| 27:I2:106:GLU:O    | 27:I2:108:LYS:NZ   | 2.18                     | 0.73              |
| 55:e2:36:MET:CA    | 55:e2:77:LYS:HE3   | 2.05                     | 0.73              |
| 1:A1:274:ASN:HB3   | 1:A1:309:THR:OG1   | 1.89                     | 0.73              |
| 5:Q1:134:ILE:O     | 5:Q1:135:LEU:HD23  | 1.89                     | 0.73              |
| 17:82:424:ILE:CD1  | 19:A2:76:ARG:HH21  | 2.01                     | 0.73              |
| 1:A1:163:LEU:HD12  | 1:A1:163:LEU:O     | 1.88                     | 0.73              |
| 1:A1:262:TRP:CD2   | 1:A1:385:THR:HG23  | 2.24                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B1:328:SER:HB3  | 2:B1:336:VAL:HG21 | 1.69                     | 0.73              |
| 2:N1:67:HIS:CD2   | 2:N1:144:LEU:HD22 | 2.21                     | 0.73              |
| 3:O1:147:THR:HG21 | 3:O1:165:TRP:NE1  | 2.03                     | 0.73              |
| 9:U1:70:LEU:CD2   | 9:U1:73:PRO:HD2   | 2.17                     | 0.73              |
| 2:B1:182:ARG:NH1  | 2:B1:185:LYS:HG2  | 2.03                     | 0.73              |
| 3:O1:22:PRO:HG2   | 7:S1:3:GLN:HB3    | 1.69                     | 0.73              |
| 62:G3:54:ARG:HD3  | 62:G3:54:ARG:N    | 2.04                     | 0.73              |
| 3:C1:30:TRP:O     | 3:C1:33:PHE:HD2   | 1.71                     | 0.73              |
| 18:92:44:THR:OG1  | 19:A2:209:TYR:CE2 | 2.42                     | 0.73              |
| 20:B2:82:LEU:HD11 | 52:12:126:LYS:CE  | 2.19                     | 0.73              |
| 62:G3:5:LYS:HZ3   | 62:G3:5:LYS:HB3   | 1.54                     | 0.73              |
| 2:B1:395:PRO:O    | 2:B1:398:VAL:HB   | 1.88                     | 0.73              |
| 4:D1:41:HIS:CD2   | 4:D1:113:LEU:HD11 | 2.24                     | 0.73              |
| 2:N1:24:LEU:CG    | 2:N1:38:LEU:HD11  | 2.19                     | 0.73              |
| 19:A2:238:PHE:O   | 23:E2:134:PRO:HD3 | 1.88                     | 0.73              |
| 59:D3:23:PRO:O    | 60:E3:66:ARG:HD3  | 1.89                     | 0.73              |
| 4:D1:224:ARG:CB   | 7:G1:25:ALA:HB1   | 2.14                     | 0.72              |
| 1:M1:426:GLY:N    | 1:M1:428:ILE:HG13 | 2.02                     | 0.72              |
| 4:P1:10:TYR:CE1   | 8:T1:73:LEU:HD21  | 2.23                     | 0.72              |
| 5:Q1:98:VAL:HA    | 5:Q1:134:ILE:HG22 | 1.69                     | 0.72              |
| 52:12:75:PRO:CD   | 52:12:223:PHE:CZ  | 2.67                     | 0.72              |
| 1:A1:171:SER:OG   | 1:A1:172:GLU:N    | 2.19                     | 0.72              |
| 7:S1:15:THR:HG22  | 7:S1:16:TYR:N     | 1.97                     | 0.72              |
| 11:W1:18:VAL:HB   | 11:W1:19:PRO:HD3  | 1.71                     | 0.72              |
| 1:A1:408:ARG:HH12 | 11:K1:15:ARG:NE   | 1.85                     | 0.72              |
| 2:B1:352:LEU:HB3  | 2:B1:411:ILE:HD11 | 1.70                     | 0.72              |
| 4:D1:27:ARG:HH12  | 10:J1:58:LYS:HG3  | 1.55                     | 0.72              |
| 1:A1:273:ALA:HA   | 1:A1:276:ILE:HD12 | 1.71                     | 0.72              |
| 2:B1:279:LEU:CD2  | 2:B1:295:LEU:HD13 | 2.19                     | 0.72              |
| 6:F1:28:LYS:HB3   | 6:F1:74:ILE:HD11  | 1.69                     | 0.72              |
| 18:92:110:MET:HG2 | 19:A2:194:ASP:C   | 2.14                     | 0.72              |
| 19:A2:302:LEU:HB3 | 38:U2:137:TRP:CB  | 2.19                     | 0.72              |
| 1:M1:335:MET:HE2  | 1:M1:339:GLN:HG3  | 1.72                     | 0.72              |
| 4:D1:54:VAL:O     | 4:D1:54:VAL:HG12  | 1.89                     | 0.72              |
| 5:E1:19:LEU:HD12  | 5:E1:19:LEU:O     | 1.90                     | 0.72              |
| 2:N1:46:ARG:HH12  | 2:N1:376:GLU:HG3  | 1.55                     | 0.72              |
| 3:C1:297:SER:O    | 3:C1:300:ILE:HG22 | 1.90                     | 0.72              |
| 5:Q1:121:GLN:HB2  | 5:Q1:170:ARG:HD3  | 1.71                     | 0.72              |
| 19:A2:314:LEU:O   | 38:U2:139:PRO:CB  | 2.38                     | 0.72              |
| 2:B1:56:ARG:NH2   | 2:B1:318:ASP:OD1  | 2.22                     | 0.72              |
| 1:M1:8:LEU:O      | 1:M1:11:VAL:HG23  | 1.90                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:309:THR:HG21  | 3:O1:370:GLY:HA3   | 1.70                     | 0.72              |
| 4:P1:74:PRO:HG2    | 4:P1:82:MET:SD     | 2.30                     | 0.72              |
| 3:C1:310:SER:HA    | 3:C1:374:ASN:ND2   | 1.97                     | 0.72              |
| 4:D1:43:MET:HG2    | 4:D1:46:VAL:HG23   | 1.70                     | 0.72              |
| 3:O1:51:LEU:HD11   | 3:O1:80:ARG:HA     | 1.69                     | 0.72              |
| 22:D2:113:PHE:HB2  | 22:D2:114:ARG:HE   | 1.54                     | 0.72              |
| 55:e2:77:LYS:HG3   | 55:e2:78:LEU:N     | 2.02                     | 0.72              |
| 1:A1:408:ARG:HH12  | 11:K1:15:ARG:CG    | 2.02                     | 0.72              |
| 3:C1:252:ASP:HB3   | 3:C1:253:PRO:CD    | 2.18                     | 0.72              |
| 4:D1:7:PRO:HG3     | 4:D1:126:TYR:HA    | 1.71                     | 0.71              |
| 4:P1:164:ILE:HD13  | 4:P1:182:VAL:HG12  | 1.70                     | 0.71              |
| 1:A1:100:LYS:NZ    | 1:A1:373:THR:OG1   | 2.18                     | 0.71              |
| 1:M1:67:THR:CG2    | 1:M1:70:ARG:HB2    | 2.20                     | 0.71              |
| 1:M1:262:TRP:CG    | 1:M1:385:THR:HG23  | 2.24                     | 0.71              |
| 1:M1:329:MET:SD    | 7:S1:5:GLY:HA3     | 2.31                     | 0.71              |
| 2:N1:277:HIS:NE2   | 2:N1:364:LEU:HD13  | 2.05                     | 0.71              |
| 2:B1:77:THR:CG2    | 2:B1:130:PRO:HA    | 2.13                     | 0.71              |
| 6:F1:33:ARG:NH2    | 6:F1:91:GLU:OE2    | 2.22                     | 0.71              |
| 1:M1:255:ILE:HG13  | 1:M1:422:VAL:HG22  | 1.71                     | 0.71              |
| 17:82:418:GLN:NE2  | 19:A2:115:GLY:CA   | 2.44                     | 0.71              |
| 56:A3:176:MET:HE3  | 56:A3:181:THR:HG22 | 1.71                     | 0.71              |
| 4:D1:10:TYR:HE1    | 8:H1:73:LEU:CD2    | 2.03                     | 0.71              |
| 2:N1:314:ALA:HB2   | 9:U1:64:LEU:HD22   | 1.70                     | 0.71              |
| 6:R1:73:GLN:HE21   | 7:S1:32:LYS:NZ     | 1.89                     | 0.71              |
| 1:A1:41:ILE:H      | 1:A1:41:ILE:HD12   | 1.54                     | 0.71              |
| 1:A1:286:GLY:O     | 1:A1:287:GLY:C     | 2.33                     | 0.71              |
| 9:I1:70:LEU:HD12   | 9:I1:71:ASN:N      | 2.04                     | 0.71              |
| 1:M1:45:SER:OG     | 1:M1:92:ARG:HG3    | 1.91                     | 0.71              |
| 5:Q1:109:GLU:CD    | 5:Q1:167:ALA:HB3   | 2.15                     | 0.71              |
| 5:Q1:139:CYS:HB2   | 5:Q1:165:TYR:HE2   | 1.54                     | 0.71              |
| 19:A2:140:GLN:OE1  | 75:A2:801:SF4:S4   | 2.48                     | 0.71              |
| 59:D3:147:LYS:HA   | 59:D3:147:LYS:HE3  | 1.72                     | 0.71              |
| 2:B1:29:LEU:HB3    | 2:B1:30:PRO:CD     | 2.20                     | 0.71              |
| 37:T2:82:GLU:HG3   | 37:T2:84:PRO:HD2   | 1.72                     | 0.71              |
| 1:A1:21:ASN:HB3    | 1:A1:217:SER:HB3   | 1.72                     | 0.71              |
| 2:B1:251:SER:OG    | 2:B1:252:LEU:N     | 2.22                     | 0.71              |
| 2:B1:300:ALA:HA    | 2:B1:307:PHE:CZ    | 2.26                     | 0.71              |
| 69:C1:401:HEM:HBC2 | 69:C1:401:HEM:HMC1 | 1.73                     | 0.71              |
| 6:R1:59:VAL:HG11   | 7:S1:10:VAL:HG22   | 1.73                     | 0.71              |
| 4:D1:150:ASN:OD1   | 4:D1:151:PRO:HD2   | 1.89                     | 0.71              |
| 3:O1:237:LEU:HD13  | 4:P1:212:MET:HG2   | 1.73                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:P1:7:PRO:HG3    | 4:P1:126:TYR:HA    | 1.73                     | 0.71              |
| 2:B1:429:ASN:ND2  | 2:N1:60:SER:HB3    | 1.98                     | 0.71              |
| 3:C1:100:ARG:NH2  | 69:C1:402:HEM:HBD1 | 2.05                     | 0.71              |
| 18:92:110:MET:HE2 | 19:A2:196:GLY:N    | 2.05                     | 0.71              |
| 17:82:381:GLN:C   | 19:A2:74:ASN:HB2   | 2.15                     | 0.70              |
| 19:A2:427:LEU:N   | 25:G2:169:ARG:HH12 | 1.89                     | 0.70              |
| 2:B1:162:ASN:ND2  | 2:B1:244:ILE:HG21  | 2.06                     | 0.70              |
| 2:B1:283:PRO:HG3  | 9:I1:55:LEU:CD2    | 2.18                     | 0.70              |
| 3:C1:147:THR:HG21 | 3:C1:165:TRP:NE1   | 2.06                     | 0.70              |
| 2:N1:68:LEU:HD11  | 2:N1:140:LEU:HD23  | 1.71                     | 0.70              |
| 19:A2:162:ASP:O   | 27:I2:105:LYS:NZ   | 2.22                     | 0.70              |
| 1:A1:233:PRO:HG2  | 5:E1:23:LYS:CD     | 2.20                     | 0.70              |
| 2:B1:384:SER:HB2  | 9:I1:62:ARG:HG2    | 1.71                     | 0.70              |
| 3:C1:110:LEU:HG   | 3:C1:114:ASN:HD21  | 1.55                     | 0.70              |
| 18:92:42:ARG:NH2  | 19:A2:199:GLY:CA   | 2.53                     | 0.70              |
| 2:B1:162:ASN:O    | 2:B1:244:ILE:HD12  | 1.89                     | 0.70              |
| 4:D1:102:ARG:HA   | 4:D1:108:ALA:O     | 1.91                     | 0.70              |
| 5:E1:15:ARG:HB2   | 5:E1:16:PRO:CD     | 2.21                     | 0.70              |
| 10:J1:49:GLY:HA2  | 10:J1:54:HIS:CB    | 2.20                     | 0.70              |
| 2:N1:140:LEU:O    | 2:N1:141:GLN:C     | 2.35                     | 0.70              |
| 3:O1:5:ARG:O      | 3:O1:9:PRO:HD2     | 1.90                     | 0.70              |
| 3:O1:47:THR:HG21  | 3:O1:83:HIS:HB2    | 1.73                     | 0.70              |
| 3:O1:218:ILE:HD13 | 4:P1:230:LEU:CD1   | 2.22                     | 0.70              |
| 3:O1:280:ILE:HD13 | 3:O1:335:LEU:HD22  | 1.72                     | 0.70              |
| 19:A2:313:LEU:N   | 38:U2:142:THR:HA   | 2.05                     | 0.70              |
| 19:A2:314:LEU:O   | 38:U2:139:PRO:HB2  | 1.91                     | 0.70              |
| 3:C1:156:ILE:HG12 | 3:C1:157:GLY:H     | 1.56                     | 0.70              |
| 3:C1:174:THR:CG2  | 3:C1:178:PHE:HE1   | 2.03                     | 0.70              |
| 4:D1:50:HIS:HB3   | 4:D1:54:VAL:CB     | 2.22                     | 0.70              |
| 4:D1:165:TYR:CZ   | 4:D1:168:VAL:HG22  | 2.27                     | 0.70              |
| 9:I1:78:TYR:OXT   | 9:I1:78:TYR:CD1    | 2.43                     | 0.70              |
| 2:N1:352:LEU:HB3  | 2:N1:411:ILE:HD11  | 1.73                     | 0.70              |
| 1:A1:60:GLU:OE2   | 1:A1:88:ALA:O      | 2.09                     | 0.70              |
| 1:A1:351:GLU:OE2  | 1:A1:403:ASP:OD1   | 2.10                     | 0.70              |
| 2:N1:51:ILE:HD13  | 2:N1:199:PHE:CG    | 2.26                     | 0.70              |
| 4:P1:11:PRO:O     | 8:T1:74:PHE:CE2    | 2.45                     | 0.70              |
| 5:Q1:95:PRO:HG2   | 5:Q1:145:VAL:HG22  | 1.74                     | 0.70              |
| 2:B1:237:ALA:HB2  | 2:B1:318:ASP:OD2   | 1.92                     | 0.70              |
| 1:M1:274:ASN:HB3  | 1:M1:309:THR:OG1   | 1.91                     | 0.70              |
| 2:N1:182:ARG:NH1  | 2:N1:185:LYS:HG2   | 2.06                     | 0.70              |
| 2:N1:212:SER:OG   | 2:N1:215:VAL:HB    | 1.92                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:S2:200:PRO:HG3  | 36:S2:223:GLN:NE2 | 2.01                     | 0.70              |
| 47:d2:25:PHE:HZ    | 47:d2:42:THR:O    | 1.75                     | 0.70              |
| 1:A1:298:ALA:HA    | 1:A1:303:LEU:HB2  | 1.73                     | 0.70              |
| 2:B1:83:PHE:CE2    | 2:B1:87:ARG:HG3   | 2.27                     | 0.70              |
| 2:B1:277:HIS:NE2   | 2:B1:364:LEU:HD13 | 2.07                     | 0.70              |
| 1:M1:236:PHE:HE2   | 1:M1:258:GLU:HB3  | 1.51                     | 0.70              |
| 6:R1:73:GLN:NE2    | 7:S1:32:LYS:HZ1   | 1.89                     | 0.70              |
| 2:B1:46:ARG:HH12   | 2:B1:376:GLU:HG3  | 1.57                     | 0.70              |
| 3:C1:18:PHE:O      | 3:C1:220:PHE:CD2  | 2.45                     | 0.70              |
| 3:O1:27:ILE:HG22   | 3:O1:27:ILE:O     | 1.91                     | 0.70              |
| 4:P1:74:PRO:CB     | 4:P1:79:GLU:HB2   | 2.19                     | 0.70              |
| 5:Q1:34:GLY:HA2    | 10:V1:10:TYR:HD1  | 1.57                     | 0.70              |
| 5:Q1:118:ARG:HH11  | 5:Q1:171:ILE:HG12 | 1.55                     | 0.70              |
| 5:Q1:171:ILE:HG22  | 5:Q1:179:ASN:OD1  | 1.92                     | 0.70              |
| 6:R1:96:GLU:O      | 6:R1:97:VAL:C     | 2.32                     | 0.70              |
| 19:A2:238:PHE:HB3  | 23:E2:140:ARG:HB3 | 1.72                     | 0.70              |
| 2:B1:166:ALA:HB2   | 2:B1:244:ILE:HG13 | 1.74                     | 0.70              |
| 3:C1:122:THR:HG22  | 3:C1:189:ILE:HD11 | 1.72                     | 0.70              |
| 4:D1:51:LEU:HA     | 4:D1:56:TYR:O     | 1.91                     | 0.70              |
| 5:Q1:185:TYR:HB3   | 5:Q1:195:VAL:HG13 | 1.74                     | 0.70              |
| 19:A2:422:TRP:C    | 25:G2:169:ARG:HD2 | 2.12                     | 0.70              |
| 3:C1:26:ASN:HD21   | 3:C1:207:ASN:CB   | 2.01                     | 0.69              |
| 7:S1:15:THR:CG2    | 7:S1:16:TYR:N     | 2.51                     | 0.69              |
| 58:C3:156:ARG:HH11 | 58:C3:156:ARG:HG3 | 1.56                     | 0.69              |
| 2:B1:129:ALA:N     | 2:B1:130:PRO:CD   | 2.55                     | 0.69              |
| 2:N1:78:LYS:HB3    | 2:N1:129:ALA:HB1  | 1.73                     | 0.69              |
| 4:D1:82:MET:SD     | 4:D1:86:LYS:HD2   | 2.32                     | 0.69              |
| 3:O1:225:THR:O     | 3:O1:229:ILE:HD12 | 1.92                     | 0.69              |
| 4:P1:158:ILE:HD11  | 4:P1:160:MET:HB2  | 1.73                     | 0.69              |
| 1:A1:162:PRO:O     | 1:A1:165:GLN:HG2  | 1.93                     | 0.69              |
| 1:A1:379:ILE:HD12  | 1:A1:390:ILE:CD1  | 2.22                     | 0.69              |
| 4:D1:94:PRO:HB2    | 4:D1:95:TYR:CD1   | 2.27                     | 0.69              |
| 2:N1:258:VAL:HG11  | 2:N1:321:LEU:HB3  | 1.74                     | 0.69              |
| 4:P1:10:TYR:CE1    | 8:T1:73:LEU:CD2   | 2.75                     | 0.69              |
| 5:Q1:158:CYS:SG    | 5:Q1:158:CYS:O    | 2.50                     | 0.69              |
| 56:A3:11:ASN:HD22  | 56:A3:14:ASP:H    | 1.39                     | 0.69              |
| 5:E1:13:TYR:O      | 7:G1:23:GLN:HB3   | 1.91                     | 0.69              |
| 7:G1:34:ILE:CB     | 7:G1:35:PRO:HD3   | 2.18                     | 0.69              |
| 1:M1:5:ALA:O       | 1:M1:8:LEU:HB2    | 1.93                     | 0.69              |
| 1:M1:316:ASP:N     | 1:M1:316:ASP:OD1  | 2.24                     | 0.69              |
| 1:M1:403:ASP:CB    | 1:M1:406:VAL:HG23 | 2.19                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:N1:338:LYS:HG2  | 2:N1:439:LEU:HD21  | 1.73                     | 0.69              |
| 3:O1:119:LEU:HD23 | 69:O1:402:HEM:C4B  | 2.28                     | 0.69              |
| 4:P1:97:ASN:OD1   | 4:P1:98:PRO:HD2    | 1.93                     | 0.69              |
| 4:P1:27:ARG:NH1   | 10:V1:58:LYS:NZ    | 2.41                     | 0.69              |
| 1:A1:32:GLN:CG    | 1:A1:33:PRO:HD2    | 2.22                     | 0.69              |
| 2:N1:165:ALA:HA   | 2:N1:173:ALA:HB1   | 1.73                     | 0.69              |
| 3:O1:156:ILE:HG13 | 3:O1:157:GLY:H     | 1.58                     | 0.69              |
| 5:Q1:136:ILE:O    | 5:Q1:136:ILE:HG22  | 1.93                     | 0.69              |
| 20:B2:92:HIS:CE1  | 20:B2:141:TYR:HE2  | 2.10                     | 0.69              |
| 56:A3:69:MET:HE2  | 56:A3:70:VAL:HG23  | 1.74                     | 0.69              |
| 1:A1:426:GLY:HA2  | 1:A1:428:ILE:N     | 2.08                     | 0.69              |
| 2:B1:34:VAL:HG11  | 2:B1:386:ALA:HB1   | 1.74                     | 0.69              |
| 3:C1:79:ILE:HG12  | 5:E1:58:PHE:HE1    | 1.57                     | 0.69              |
| 7:G1:73:ASN:N     | 7:G1:74:PRO:CD     | 2.55                     | 0.69              |
| 1:M1:145:MET:SD   | 1:M1:248:LEU:HD12  | 2.32                     | 0.69              |
| 1:M1:365:LEU:HD21 | 1:M1:395:TRP:CD1   | 2.27                     | 0.69              |
| 2:N1:319:SER:OG   | 2:N1:320:GLY:N     | 2.26                     | 0.69              |
| 3:O1:129:MET:HG2  | 3:O1:178:PHE:CD1   | 2.27                     | 0.69              |
| 4:P1:220:TYR:CE2  | 7:S1:26:PHE:CE1    | 2.81                     | 0.69              |
| 5:Q1:68:VAL:HG12  | 5:Q1:69:LEU:N      | 2.08                     | 0.69              |
| 5:Q1:114:VAL:HG12 | 5:Q1:115:SER:N     | 2.08                     | 0.69              |
| 19:A2:312:GLY:H   | 38:U2:143:PRO:C    | 2.01                     | 0.69              |
| 2:B1:247:GLN:HE22 | 2:B1:429:ASN:ND2   | 1.91                     | 0.69              |
| 3:C1:135:TRP:HH2  | 3:C1:170:VAL:HG12  | 1.57                     | 0.69              |
| 4:D1:176:PRO:HB2  | 4:D1:181:GLN:NE2   | 2.06                     | 0.69              |
| 2:N1:47:ILE:HG22  | 2:N1:48:GLY:N      | 2.08                     | 0.69              |
| 3:O1:103:TYR:O    | 3:O1:315:MET:HB2   | 1.93                     | 0.69              |
| 19:A2:426:ASP:C   | 25:G2:169:ARG:HH12 | 2.00                     | 0.69              |
| 1:M1:278:GLY:O    | 1:M1:309:THR:HG23  | 1.93                     | 0.69              |
| 1:M1:304:CYS:HB3  | 1:M1:334:MET:SD    | 2.33                     | 0.69              |
| 3:O1:15:ASN:ND2   | 3:O1:18:PHE:CE2    | 2.60                     | 0.69              |
| 7:S1:2:ARG:HB2    | 7:S1:6:HIS:HD2     | 1.58                     | 0.69              |
| 55:e2:67:ASP:O    | 55:e2:68:ASP:C     | 2.35                     | 0.69              |
| 58:C3:12:ASN:HD22 | 65:J3:20:VAL:H     | 1.39                     | 0.69              |
| 2:B1:308:ASP:OD1  | 2:B1:309:VAL:N     | 2.26                     | 0.68              |
| 3:C1:132:VAL:HA   | 3:C1:139:SER:HB3   | 1.74                     | 0.68              |
| 3:C1:177:ARG:NH2  | 5:Q1:62:MET:O      | 2.23                     | 0.68              |
| 1:M1:343:MET:HE1  | 1:M1:416:TYR:HD2   | 1.57                     | 0.68              |
| 3:O1:79:ILE:HG12  | 5:Q1:58:PHE:HE1    | 1.59                     | 0.68              |
| 4:P1:158:ILE:HD13 | 4:P1:160:MET:CB    | 2.22                     | 0.68              |
| 4:P1:236:ALA:HB3  | 7:S1:14:ILE:HB     | 1.76                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Q1:83:GLU:HG3   | 5:Q1:100:HIS:NE2   | 2.08                     | 0.68              |
| 55:e2:75:TYR:CB   | 55:e2:78:LEU:CB    | 2.69                     | 0.68              |
| 57:B3:13:THR:HB   | 57:B3:168:LEU:HD23 | 1.74                     | 0.68              |
| 1:A1:244:ARG:HG2  | 7:G1:10:VAL:HG12   | 1.74                     | 0.68              |
| 4:D1:97:ASN:OD1   | 4:D1:98:PRO:HD2    | 1.92                     | 0.68              |
| 2:N1:100:SER:HB3  | 2:N1:105:MET:HG3   | 1.74                     | 0.68              |
| 3:O1:252:ASP:HB3  | 3:O1:253:PRO:CD    | 2.23                     | 0.68              |
| 1:A1:39:VAL:HG11  | 1:A1:117:VAL:HG21  | 1.73                     | 0.68              |
| 1:A1:341:GLN:OE1  | 1:A1:344:ARG:NH1   | 2.25                     | 0.68              |
| 1:M1:245:GLU:OE1  | 1:M1:248:LEU:HD23  | 1.92                     | 0.68              |
| 1:M1:389:ARG:O    | 1:M1:390:ILE:HD13  | 1.94                     | 0.68              |
| 2:N1:300:ALA:HA   | 2:N1:307:PHE:CZ    | 2.28                     | 0.68              |
| 4:P1:102:ARG:HA   | 4:P1:108:ALA:O     | 1.92                     | 0.68              |
| 5:Q1:121:GLN:HB2  | 5:Q1:170:ARG:CD    | 2.24                     | 0.68              |
| 8:T1:65:ARG:HG3   | 8:T1:66:ASP:N      | 2.09                     | 0.68              |
| 1:A1:408:ARG:NH1  | 11:K1:15:ARG:HG2   | 2.09                     | 0.68              |
| 1:A1:445:ARG:O    | 1:A1:446:PHE:HB2   | 1.93                     | 0.68              |
| 2:B1:348:ALA:HB1  | 2:B1:415:LYS:HA    | 1.76                     | 0.68              |
| 3:C1:234:LEU:HD23 | 4:D1:216:LEU:HD21  | 1.74                     | 0.68              |
| 8:H1:22:GLU:O     | 8:H1:25:GLU:HG2    | 1.94                     | 0.68              |
| 1:M1:21:ASN:CB    | 1:M1:217:SER:HB3   | 2.22                     | 0.68              |
| 1:M1:351:GLU:OE2  | 1:M1:403:ASP:OD1   | 2.10                     | 0.68              |
| 6:R1:75:LEU:HD12  | 6:R1:76:PRO:CD     | 2.23                     | 0.68              |
| 2:B1:62:ASN:ND2   | 2:B1:65:THR:OG1    | 2.26                     | 0.68              |
| 4:D1:134:TYR:HE2  | 4:D1:163:PRO:HG2   | 1.58                     | 0.68              |
| 4:D1:237:TYR:CE2  | 4:D1:239:PRO:HG3   | 2.29                     | 0.68              |
| 4:P1:211:MET:HE1  | 10:V1:31:PHE:CZ    | 2.28                     | 0.68              |
| 19:A2:367:CYS:SG  | 19:A2:368:THR:N    | 2.66                     | 0.68              |
| 55:e2:67:ASP:O    | 55:e2:69:GLY:N     | 2.26                     | 0.68              |
| 3:C1:245:PHE:CD1  | 4:D1:17:LEU:HD13   | 2.27                     | 0.68              |
| 6:R1:75:LEU:O     | 6:R1:80:TRP:NE1    | 2.27                     | 0.68              |
| 2:B1:135:TRP:CD2  | 6:R1:49:ARG:HD3    | 2.29                     | 0.68              |
| 1:M1:46:ARG:HH22  | 1:M1:316:ASP:CG    | 2.02                     | 0.68              |
| 5:Q1:76:ILE:HG22  | 5:Q1:193:VAL:C     | 2.19                     | 0.68              |
| 6:R1:51:PRO:HG2   | 6:R1:54:LEU:HD22   | 1.74                     | 0.68              |
| 5:E1:18:VAL:HG11  | 5:E1:32:ARG:NH1    | 2.09                     | 0.68              |
| 1:M1:236:PHE:CD2  | 1:M1:258:GLU:HG2   | 2.28                     | 0.68              |
| 4:P1:5:LEU:HB3    | 4:P1:152:TYR:CD1   | 2.28                     | 0.68              |
| 5:Q1:171:ILE:HG23 | 5:Q1:171:ILE:O     | 1.94                     | 0.68              |
| 7:S1:51:PRO:O     | 7:S1:54:ALA:HB3    | 1.94                     | 0.68              |
| 10:V1:22:LEU:O    | 10:V1:26:VAL:HG23  | 1.93                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A1:151:ASN:ND2  | 5:E1:2:HIS:NE2     | 2.42                     | 0.68              |
| 1:A1:350:THR:HB   | 1:A1:353:GLU:CG    | 2.24                     | 0.68              |
| 1:A1:426:GLY:N    | 1:A1:428:ILE:HG13  | 2.06                     | 0.68              |
| 3:C1:311:LYS:HD2  | 3:C1:379:TRP:HB3   | 1.76                     | 0.68              |
| 3:O1:100:ARG:NH2  | 69:O1:402:HEM:HBD1 | 2.04                     | 0.68              |
| 27:I2:106:GLU:OE1 | 27:I2:106:GLU:N    | 2.27                     | 0.68              |
| 1:A1:67:THR:HG22  | 1:A1:70:ARG:HB2    | 1.76                     | 0.68              |
| 1:A1:80:GLU:O     | 1:A1:83:GLY:N      | 2.26                     | 0.68              |
| 1:A1:365:LEU:HD21 | 1:A1:395:TRP:CD1   | 2.29                     | 0.68              |
| 3:C1:174:THR:O    | 3:C1:178:PHE:HD1   | 1.77                     | 0.68              |
| 5:E1:60:SER:HA    | 5:E1:63:SER:OG     | 1.94                     | 0.68              |
| 1:M1:39:VAL:HG12  | 1:M1:41:ILE:CD1    | 2.23                     | 0.68              |
| 4:P1:27:ARG:NH1   | 10:V1:58:LYS:HZ2   | 1.91                     | 0.68              |
| 3:C1:244:LEU:HD23 | 4:D1:205:GLY:HA2   | 1.76                     | 0.67              |
| 1:M1:4:TYR:CZ     | 1:M1:8:LEU:HD11    | 2.28                     | 0.67              |
| 2:N1:264:ILE:CG2  | 2:N1:317:SER:HA    | 2.23                     | 0.67              |
| 60:E3:43:PRO:HB2  | 60:E3:48:ILE:HD11  | 1.76                     | 0.67              |
| 67:L3:19:TRP:HZ2  | 68:M3:14:GLU:HG2   | 1.59                     | 0.67              |
| 3:C1:108:THR:HB   | 3:C1:313:ARG:HH11  | 1.58                     | 0.67              |
| 3:C1:109:PHE:O    | 3:C1:110:LEU:C     | 2.36                     | 0.67              |
| 1:A1:158:PHE:CE1  | 1:A1:317:THR:HG21  | 2.28                     | 0.67              |
| 3:C1:22:PRO:HG2   | 7:G1:3:GLN:HB3     | 1.76                     | 0.67              |
| 1:M1:86:LEU:HD13  | 1:M1:99:ILE:HG12   | 1.75                     | 0.67              |
| 1:M1:408:ARG:HH12 | 11:W1:15:ARG:CG    | 2.07                     | 0.67              |
| 3:O1:177:ARG:O    | 3:O1:181:PHE:CD2   | 2.47                     | 0.67              |
| 3:O1:244:LEU:O    | 4:P1:201:ARG:HD3   | 1.95                     | 0.67              |
| 3:C1:244:LEU:O    | 4:D1:201:ARG:HD3   | 1.95                     | 0.67              |
| 5:E1:53:ASN:OD1   | 5:E1:53:ASN:N      | 2.27                     | 0.67              |
| 6:F1:51:PRO:HD3   | 2:N1:134:ARG:HH12  | 1.57                     | 0.67              |
| 7:G1:50:PRO:CB    | 7:G1:51:PRO:HD3    | 2.24                     | 0.67              |
| 17:82:211:ALA:HB2 | 17:82:223:PRO:HB3  | 1.76                     | 0.67              |
| 63:H3:38:ARG:HG2  | 63:H3:85:ILE:HG23  | 1.76                     | 0.67              |
| 4:D1:208:MET:HE2  | 4:D1:208:MET:O     | 1.95                     | 0.67              |
| 5:E1:68:VAL:HG12  | 5:E1:69:LEU:N      | 2.10                     | 0.67              |
| 9:I1:53:GLU:O     | 9:I1:55:LEU:HG     | 1.94                     | 0.67              |
| 17:82:422:HIS:ND1 | 19:A2:79:LEU:HD13  | 2.10                     | 0.67              |
| 20:B2:163:PRO:HG2 | 20:B2:168:GLN:HE21 | 1.59                     | 0.67              |
| 52:12:120:GLY:O   | 52:12:128:ALA:O    | 2.12                     | 0.67              |
| 1:A1:408:ARG:NH1  | 11:K1:15:ARG:CG    | 2.57                     | 0.67              |
| 2:N1:156:GLN:HE22 | 9:U1:56:ARG:HD3    | 1.58                     | 0.67              |
| 5:Q1:89:PHE:HB2   | 5:Q1:96:LEU:HB3    | 1.76                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:A2:313:LEU:CD2 | 38:U2:142:THR:CA   | 2.72                     | 0.67              |
| 56:A3:151:HIS:O   | 56:A3:155:VAL:HG23 | 1.95                     | 0.67              |
| 58:C3:154:GLY:HA2 | 61:F3:6:VAL:HG22   | 1.75                     | 0.67              |
| 1:A1:426:GLY:HA2  | 1:A1:427:PRO:C     | 2.19                     | 0.67              |
| 2:N1:209:LEU:CD2  | 2:N1:375:SER:HB2   | 2.25                     | 0.67              |
| 3:O1:244:LEU:HD11 | 4:P1:204:MET:HE2   | 1.75                     | 0.67              |
| 18:92:224:SER:OG  | 18:92:226:GLU:CG   | 2.43                     | 0.67              |
| 1:A1:241:ILE:HG13 | 7:G1:16:TYR:CD1    | 2.30                     | 0.67              |
| 3:C1:234:LEU:CD2  | 4:D1:216:LEU:HD21  | 2.24                     | 0.67              |
| 3:C1:332:LEU:HD21 | 3:C1:358:TYR:HE1   | 1.60                     | 0.67              |
| 7:S1:71:ARG:HH21  | 8:T1:60:ASP:CG     | 2.02                     | 0.67              |
| 19:A2:311:LYS:CB  | 38:U2:142:THR:O    | 2.43                     | 0.67              |
| 52:12:126:LYS:CD  | 52:12:127:TYR:H    | 1.98                     | 0.67              |
| 3:O1:22:PRO:CG    | 7:S1:3:GLN:HB3     | 2.25                     | 0.67              |
| 4:P1:32:VAL:HG11  | 4:P1:186:VAL:HG22  | 1.76                     | 0.67              |
| 1:A1:53:ASN:OD1   | 1:A1:170:PRO:HD3   | 1.95                     | 0.67              |
| 1:A1:251:ALA:O    | 1:A1:325:VAL:HA    | 1.95                     | 0.67              |
| 1:M1:80:GLU:O     | 1:M1:83:GLY:N      | 2.28                     | 0.67              |
| 9:U1:70:LEU:CD1   | 9:U1:72:VAL:H      | 2.08                     | 0.67              |
| 1:A1:324:PHE:CD1  | 1:A1:334:MET:HG2   | 2.30                     | 0.66              |
| 3:C1:56:THR:HG21  | 3:O1:58:ASP:OD2    | 1.94                     | 0.66              |
| 8:H1:73:LEU:HD21  | 8:H1:74:PHE:HD1    | 1.58                     | 0.66              |
| 1:M1:27:SER:HA    | 1:M1:199:ALA:O     | 1.94                     | 0.66              |
| 1:M1:405:ARG:O    | 1:M1:409:GLU:HG3   | 1.96                     | 0.66              |
| 2:N1:283:PRO:HG3  | 9:U1:55:LEU:CD2    | 2.24                     | 0.66              |
| 2:N1:394:PRO:O    | 2:N1:398:VAL:HG23  | 1.94                     | 0.66              |
| 19:A2:313:LEU:CG  | 38:U2:142:THR:HA   | 2.24                     | 0.66              |
| 1:A1:346:CYS:CB   | 1:A1:412:SER:OG    | 2.44                     | 0.66              |
| 4:D1:75:ASN:ND2   | 4:D1:80:MET:O      | 2.28                     | 0.66              |
| 6:F1:42:ASP:OD2   | 6:F1:101:ARG:NH1   | 2.28                     | 0.66              |
| 4:P1:82:MET:SD    | 4:P1:86:LYS:HD2    | 2.35                     | 0.66              |
| 19:A2:111:LYS:CE  | 33:P2:53:TYR:HE2   | 2.07                     | 0.66              |
| 3:C1:169:SER:CB   | 5:Q1:93:GLY:HA3    | 2.24                     | 0.66              |
| 2:N1:327:ILE:O    | 2:N1:327:ILE:HG22  | 1.95                     | 0.66              |
| 3:O1:122:THR:HG21 | 3:O1:189:ILE:HG12  | 1.78                     | 0.66              |
| 4:P1:138:PRO:HB3  | 8:T1:55:THR:N      | 2.10                     | 0.66              |
| 6:R1:28:LYS:HD2   | 6:R1:74:ILE:CD1    | 2.24                     | 0.66              |
| 57:B3:186:SER:HB3 | 57:B3:213:LEU:HD22 | 1.75                     | 0.66              |
| 3:C1:156:ILE:O    | 3:C1:157:GLY:C     | 2.39                     | 0.66              |
| 4:D1:10:TYR:HE1   | 8:H1:73:LEU:HD21   | 1.60                     | 0.66              |
| 1:M1:236:PHE:HD2  | 1:M1:258:GLU:HG2   | 1.60                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:408:ARG:CZ    | 11:W1:15:ARG:HE    | 2.08                     | 0.66              |
| 3:O1:200:LEU:HG    | 3:O1:200:LEU:O     | 1.95                     | 0.66              |
| 3:O1:267:HIS:NE2   | 3:O1:269:LYS:HD3   | 2.10                     | 0.66              |
| 17:82:383:THR:HG21 | 19:A2:75:CYS:HA    | 1.76                     | 0.66              |
| 18:92:137:THR:H    | 18:92:140:CYS:HB2  | 1.60                     | 0.66              |
| 27:I2:105:LYS:HG3  | 27:I2:105:LYS:O    | 1.96                     | 0.66              |
| 2:B1:31:ASN:HB3    | 2:B1:201:SER:HB3   | 1.78                     | 0.66              |
| 2:N1:134:ARG:HG2   | 2:N1:135:TRP:N     | 2.11                     | 0.66              |
| 2:N1:159:VAL:HG23  | 2:N1:427:SER:OG    | 1.95                     | 0.66              |
| 3:O1:72:ASP:OD1    | 4:P1:49:ARG:NH1    | 2.25                     | 0.66              |
| 3:O1:124:MET:HE1   | 3:O1:298:ILE:HG21  | 1.77                     | 0.66              |
| 3:O1:156:ILE:O     | 3:O1:157:GLY:C     | 2.39                     | 0.66              |
| 3:O1:359:PHE:O     | 3:O1:363:LEU:HB2   | 1.95                     | 0.66              |
| 4:P1:26:ILE:HG22   | 4:P1:54:VAL:HG13   | 1.78                     | 0.66              |
| 58:C3:209:ILE:O    | 58:C3:213:THR:HG23 | 1.95                     | 0.66              |
| 3:C1:240:MET:HA    | 3:C1:243:VAL:CG1   | 2.24                     | 0.66              |
| 4:D1:220:TYR:CE2   | 7:G1:26:PHE:CE1    | 2.83                     | 0.66              |
| 2:N1:129:ALA:N     | 2:N1:130:PRO:CD    | 2.58                     | 0.66              |
| 2:N1:132:PHE:HB3   | 2:N1:137:VAL:HG21  | 1.76                     | 0.66              |
| 2:N1:148:LYS:HG3   | 2:N1:177:TYR:HB3   | 1.76                     | 0.66              |
| 2:N1:180:ASP:O     | 2:N1:183:ILE:HD12  | 1.95                     | 0.66              |
| 5:Q1:126:ARG:NH2   | 5:Q1:168:SER:O     | 2.23                     | 0.66              |
| 10:J1:36:ASP:O     | 10:J1:37:GLN:C     | 2.35                     | 0.66              |
| 1:M1:236:PHE:CD2   | 1:M1:258:GLU:HB3   | 2.30                     | 0.66              |
| 3:O1:8:HIS:HB3     | 3:O1:9:PRO:HD3     | 1.76                     | 0.66              |
| 3:O1:26:ASN:ND2    | 3:O1:208:PRO:HD2   | 2.11                     | 0.66              |
| 3:O1:345:HIS:HB3   | 3:O1:346:PRO:CD    | 2.21                     | 0.66              |
| 1:A1:236:PHE:CD2   | 1:A1:258:GLU:HB3   | 2.31                     | 0.66              |
| 1:A1:351:GLU:HA    | 1:A1:404:ALA:HB2   | 1.77                     | 0.66              |
| 1:M1:91:THR:HG23   | 1:M1:92:ARG:H      | 1.60                     | 0.66              |
| 1:M1:426:GLY:HA2   | 1:M1:428:ILE:HG13  | 1.72                     | 0.66              |
| 2:N1:191:LEU:O     | 2:N1:195:VAL:HG23  | 1.94                     | 0.66              |
| 2:N1:395:PRO:O     | 2:N1:398:VAL:HB    | 1.94                     | 0.66              |
| 3:O1:32:ASN:O      | 3:O1:36:LEU:HG     | 1.95                     | 0.66              |
| 3:O1:102:LEU:HD21  | 3:O1:304:ILE:HD12  | 1.78                     | 0.66              |
| 4:P1:233:ARG:HG3   | 7:S1:17:SER:HB2    | 1.77                     | 0.66              |
| 5:Q1:1:SER:OG      | 5:Q1:1:SER:CA      | 2.44                     | 0.66              |
| 8:T1:22:GLU:O      | 8:T1:25:GLU:HG2    | 1.94                     | 0.66              |
| 19:A2:313:LEU:HD23 | 38:U2:142:THR:HA   | 1.76                     | 0.66              |
| 1:A1:143:THR:O     | 1:A1:143:THR:HG23  | 1.94                     | 0.66              |
| 1:A1:331:ILE:HD11  | 1:A1:427:PRO:O     | 1.96                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:S1:73:ASN:N      | 7:S1:74:PRO:CD     | 2.58                     | 0.66              |
| 10:V1:35:PHE:O     | 10:V1:36:ASP:C     | 2.37                     | 0.66              |
| 19:A2:159:ALA:HB3  | 27:I2:84:VAL:HG12  | 1.77                     | 0.66              |
| 19:A2:303:THR:HG23 | 38:U2:136:GLU:HA   | 1.76                     | 0.66              |
| 44:a2:79:ASN:CG    | 55:e2:76:PRO:HG3   | 2.20                     | 0.66              |
| 63:H3:39:CYS:HG    | 63:H3:53:CYS:HG    | 0.70                     | 0.66              |
| 3:C1:32:ASN:HD21   | 3:C1:228:ASP:HA    | 1.61                     | 0.66              |
| 5:E1:15:ARG:HH21   | 5:E1:32:ARG:HB2    | 1.60                     | 0.66              |
| 9:I1:70:LEU:CD1    | 9:I1:72:VAL:H      | 2.09                     | 0.66              |
| 5:Q1:188:THR:OG1   | 5:Q1:192:MET:HB2   | 1.96                     | 0.66              |
| 56:A3:298:ASP:HB2  | 56:A3:301:THR:HG23 | 1.77                     | 0.66              |
| 58:C3:160:LEU:HD13 | 58:C3:222:GLN:HG2  | 1.78                     | 0.66              |
| 1:A1:262:TRP:CG    | 1:A1:385:THR:HG23  | 2.31                     | 0.65              |
| 1:M1:161:THR:HB    | 1:M1:162:PRO:HD2   | 1.77                     | 0.65              |
| 3:O1:44:GLN:OE1    | 3:O1:83:HIS:ND1    | 2.30                     | 0.65              |
| 4:P1:27:ARG:NH1    | 10:V1:58:LYS:HG3   | 2.11                     | 0.65              |
| 19:A2:313:LEU:HG   | 38:U2:142:THR:CB   | 2.26                     | 0.65              |
| 29:K2:20:ARG:HB2   | 29:K2:66:TRP:HB2   | 1.77                     | 0.65              |
| 1:M1:163:LEU:HD12  | 1:M1:163:LEU:O     | 1.95                     | 0.65              |
| 3:O1:102:LEU:HD21  | 3:O1:304:ILE:HD13  | 1.77                     | 0.65              |
| 1:A1:78:GLU:HG2    | 1:A1:112:LEU:HD21  | 1.78                     | 0.65              |
| 3:C1:243:VAL:HG13  | 3:C1:244:LEU:HD13  | 1.77                     | 0.65              |
| 1:M1:351:GLU:OE2   | 1:M1:404:ALA:HB3   | 1.96                     | 0.65              |
| 2:N1:98:VAL:HG22   | 2:N1:107:TYR:CD2   | 2.30                     | 0.65              |
| 2:N1:247:GLN:HE22  | 2:N1:429:ASN:ND2   | 1.95                     | 0.65              |
| 2:N1:248:ASN:HB2   | 2:N1:428:GLY:CA    | 2.22                     | 0.65              |
| 3:O1:122:THR:CG2   | 3:O1:189:ILE:CD1   | 2.75                     | 0.65              |
| 3:O1:218:ILE:HD13  | 4:P1:230:LEU:HD11  | 1.78                     | 0.65              |
| 5:Q1:102:THR:O     | 5:Q1:106:ILE:HG13  | 1.96                     | 0.65              |
| 19:A2:111:LYS:HD2  | 33:P2:53:TYR:OH    | 1.96                     | 0.65              |
| 1:A1:75:LEU:HD21   | 1:A1:116:ILE:HG12  | 1.78                     | 0.65              |
| 4:D1:11:PRO:O      | 8:H1:74:PHE:CZ     | 2.49                     | 0.65              |
| 2:N1:207:ILE:CD1   | 2:N1:383:GLY:HA2   | 2.25                     | 0.65              |
| 3:O1:310:SER:CB    | 3:O1:318:ARG:NH1   | 2.59                     | 0.65              |
| 5:Q1:101:ARG:HD3   | 5:Q1:133:VAL:HG11  | 1.76                     | 0.65              |
| 10:V1:9:LEU:HD12   | 10:V1:13:LEU:HD12  | 1.77                     | 0.65              |
| 52:12:75:PRO:CA    | 52:12:223:PHE:CZ   | 2.79                     | 0.65              |
| 57:B3:120:SER:OG   | 57:B3:138:VAL:HG21 | 1.97                     | 0.65              |
| 4:D1:236:ALA:HB3   | 7:G1:14:ILE:HB     | 1.78                     | 0.65              |
| 7:G1:2:ARG:HB2     | 7:G1:6:HIS:HD2     | 1.59                     | 0.65              |
| 10:J1:55:ILE:HG23  | 10:J1:58:LYS:HE2   | 1.79                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:R1:42:ASP:OD2    | 6:R1:101:ARG:NH1  | 2.30                     | 0.65              |
| 58:C3:101:PHE:HZ   | 58:C3:260:GLY:HA3 | 1.61                     | 0.65              |
| 1:A1:106:LEU:CD2   | 1:A1:203:LEU:HD13 | 2.26                     | 0.65              |
| 1:A1:426:GLY:N     | 1:A1:428:ILE:HG12 | 2.10                     | 0.65              |
| 2:B1:56:ARG:NH2    | 2:B1:172:LEU:HD21 | 2.12                     | 0.65              |
| 2:B1:134:ARG:NH1   | 6:R1:51:PRO:HD3   | 2.11                     | 0.65              |
| 2:B1:354:ASN:N     | 2:B1:355:PRO:HD2  | 2.10                     | 0.65              |
| 4:D1:241:LYS:OXT   | 4:D1:241:LYS:HG2  | 1.95                     | 0.65              |
| 1:M1:45:SER:OG     | 1:M1:92:ARG:CG    | 2.44                     | 0.65              |
| 1:M1:335:MET:HE1   | 1:M1:338:LEU:HD23 | 1.79                     | 0.65              |
| 2:N1:156:GLN:NE2   | 9:U1:56:ARG:HD3   | 2.12                     | 0.65              |
| 2:N1:384:SER:HB2   | 9:U1:62:ARG:HG2   | 1.79                     | 0.65              |
| 5:Q1:85:LYS:HG2    | 5:Q1:86:ASN:N     | 2.11                     | 0.65              |
| 1:A1:342:TRP:O     | 1:A1:343:MET:C    | 2.38                     | 0.65              |
| 5:E1:62:MET:O      | 3:O1:177:ARG:NH2  | 2.30                     | 0.65              |
| 1:M1:298:ALA:HA    | 1:M1:303:LEU:HB2  | 1.77                     | 0.65              |
| 3:O1:315:MET:HE2   | 3:O1:318:ARG:HH21 | 1.60                     | 0.65              |
| 6:R1:73:GLN:HE21   | 7:S1:32:LYS:HZ1   | 1.44                     | 0.65              |
| 1:A1:198:ALA:O     | 1:A1:199:ALA:HB2  | 1.95                     | 0.65              |
| 3:C1:174:THR:O     | 3:C1:178:PHE:CD1  | 2.50                     | 0.65              |
| 3:C1:183:PHE:CE1   | 3:O1:183:PHE:CD1  | 2.84                     | 0.65              |
| 3:O1:311:LYS:HD2   | 3:O1:379:TRP:HB3  | 1.79                     | 0.65              |
| 4:P1:50:HIS:HB3    | 4:P1:54:VAL:CB    | 2.26                     | 0.65              |
| 5:Q1:117:LEU:O     | 5:Q1:118:ARG:C    | 2.39                     | 0.65              |
| 19:A2:157:LYS:HB2  | 27:I2:100:TYR:CE2 | 2.31                     | 0.65              |
| 21:C2:123:THR:HG21 | 25:G2:129:SER:H   | 1.62                     | 0.65              |
| 2:B1:109:VAL:HG22  | 2:B1:119:LEU:HD23 | 1.77                     | 0.65              |
| 2:B1:279:LEU:HD22  | 2:B1:295:LEU:HD13 | 1.76                     | 0.65              |
| 4:D1:178:THR:HG23  | 8:H1:15:ASP:N     | 2.11                     | 0.65              |
| 1:M1:6:GLN:O       | 1:M1:7:ALA:C      | 2.39                     | 0.65              |
| 4:P1:164:ILE:HD11  | 4:P1:186:VAL:HG21 | 1.79                     | 0.65              |
| 19:A2:422:TRP:O    | 25:G2:169:ARG:NH1 | 2.30                     | 0.65              |
| 19:A2:674:LEU:HD12 | 29:K2:46:LYS:CD   | 2.26                     | 0.65              |
| 1:A1:158:PHE:HB2   | 1:A1:164:ALA:HB2  | 1.79                     | 0.65              |
| 3:C1:296:PHE:HD1   | 3:C1:359:PHE:HE1  | 1.45                     | 0.65              |
| 4:D1:138:PRO:HB3   | 8:H1:55:THR:N     | 2.12                     | 0.65              |
| 6:F1:28:LYS:CB     | 6:F1:74:ILE:HD11  | 2.26                     | 0.65              |
| 1:M1:38:GLY:HA3    | 1:M1:40:TRP:HZ3   | 1.62                     | 0.65              |
| 1:M1:91:THR:CG2    | 1:M1:92:ARG:N     | 2.60                     | 0.65              |
| 1:M1:391:PRO:HB2   | 1:M1:395:TRP:CZ2  | 2.32                     | 0.65              |
| 2:N1:303:VAL:HG12  | 2:N1:304:HIS:N    | 2.11                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N1:436:ILE:HD12  | 2:N1:437:ASP:OD1   | 1.96                     | 0.65              |
| 56:A3:195:LEU:HD23 | 56:A3:245:ILE:HD13 | 1.79                     | 0.65              |
| 2:B1:155:PRO:HB2   | 2:B1:254:HIS:CE1   | 2.32                     | 0.64              |
| 2:B1:333:ALA:O     | 2:B1:337:ILE:HD12  | 1.97                     | 0.64              |
| 3:C1:78:ILE:HD11   | 5:E1:57:GLN:NE2    | 2.12                     | 0.64              |
| 3:C1:270:PRO:HB2   | 3:C1:274:PHE:HB2   | 1.78                     | 0.64              |
| 3:C1:345:HIS:HB3   | 3:C1:346:PRO:HD3   | 1.79                     | 0.64              |
| 10:J1:12:LEU:HD23  | 10:J1:13:LEU:HD21  | 1.79                     | 0.64              |
| 4:P1:70:VAL:HG23   | 4:P1:84:PRO:HD3    | 1.80                     | 0.64              |
| 2:B1:257:LEU:HD13  | 2:B1:424:MET:HB2   | 1.77                     | 0.64              |
| 4:D1:229:VAL:HG22  | 7:G1:18:LEU:O      | 1.97                     | 0.64              |
| 4:D1:233:ARG:HG3   | 7:G1:17:SER:HB2    | 1.80                     | 0.64              |
| 1:M1:426:GLY:N     | 1:M1:428:ILE:CG1   | 2.60                     | 0.64              |
| 2:N1:71:LEU:HD13   | 2:N1:143:GLN:HG3   | 1.78                     | 0.64              |
| 4:P1:51:LEU:HA     | 4:P1:56:TYR:O      | 1.97                     | 0.64              |
| 2:B1:318:ASP:OD1   | 2:B1:318:ASP:N     | 2.28                     | 0.64              |
| 4:D1:27:ARG:O      | 4:D1:28:ARG:C      | 2.41                     | 0.64              |
| 1:M1:158:PHE:CZ    | 1:M1:317:THR:HG21  | 2.31                     | 0.64              |
| 1:M1:279:HIS:HA    | 1:M1:307:PHE:O     | 1.97                     | 0.64              |
| 2:N1:279:LEU:HD22  | 2:N1:344:VAL:HG22  | 1.80                     | 0.64              |
| 4:P1:54:VAL:O      | 4:P1:54:VAL:HG12   | 1.96                     | 0.64              |
| 5:Q1:91:TRP:O      | 5:Q1:92:ARG:HB2    | 1.97                     | 0.64              |
| 10:V1:51:LEU:HB3   | 10:V1:52:TRP:CZ3   | 2.32                     | 0.64              |
| 28:J2:47:LEU:HD23  | 34:Q2:22:SER:HB2   | 1.80                     | 0.64              |
| 1:A1:106:LEU:N     | 1:A1:107:PRO:HD2   | 2.11                     | 0.64              |
| 2:B1:385:GLN:HG2   | 9:I1:62:ARG:NH1    | 2.10                     | 0.64              |
| 3:C1:170:VAL:HG12  | 3:C1:170:VAL:O     | 1.97                     | 0.64              |
| 3:C1:206:ASN:CB    | 3:C1:313:ARG:HH21  | 2.05                     | 0.64              |
| 4:D1:55:CYS:SG     | 10:J1:55:ILE:HG22  | 2.37                     | 0.64              |
| 2:N1:133:ARG:HD3   | 2:N1:135:TRP:CZ2   | 2.33                     | 0.64              |
| 5:Q1:76:ILE:HD12   | 5:Q1:192:MET:CE    | 2.28                     | 0.64              |
| 19:A2:111:LYS:HE2  | 33:P2:53:TYR:HE2   | 1.62                     | 0.64              |
| 1:A1:269:ALA:HB3   | 1:A1:410:VAL:HG11  | 1.80                     | 0.64              |
| 2:B1:128:THR:HG23  | 2:B1:226:ILE:HD11  | 1.80                     | 0.64              |
| 3:C1:240:MET:O     | 3:C1:244:LEU:HB2   | 1.96                     | 0.64              |
| 4:D1:178:THR:HG21  | 8:H1:16:PRO:HG2    | 1.79                     | 0.64              |
| 3:O1:296:PHE:HD1   | 3:O1:359:PHE:HE1   | 1.43                     | 0.64              |
| 55:e2:70:THR:C     | 55:e2:72:TYR:H     | 2.01                     | 0.64              |
| 2:B1:253:VAL:HG23  | 2:B1:427:SER:O     | 1.96                     | 0.64              |
| 3:C1:264:THR:CG2   | 5:Q1:144:CYS:HB3   | 2.24                     | 0.64              |
| 1:M1:436:ARG:HE    | 3:O1:222:PRO:HD3   | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:R1:73:GLN:HA    | 7:S1:39:ARG:HH21  | 1.61                     | 0.64              |
| 17:82:386:ARG:HD2 | 19:A2:178:GLN:OE1 | 1.97                     | 0.64              |
| 52:12:25:ARG:HG2  | 52:12:25:ARG:NH1  | 2.10                     | 0.64              |
| 62:G3:5:LYS:HZ3   | 62:G3:6:GLY:N     | 1.86                     | 0.64              |
| 2:B1:200:THR:CG2  | 2:B1:203:ARG:HD2  | 2.23                     | 0.64              |
| 1:M1:408:ARG:NH1  | 11:W1:15:ARG:CG   | 2.61                     | 0.64              |
| 3:O1:172:LYS:O    | 3:O1:173:ALA:C    | 2.41                     | 0.64              |
| 3:O1:207:ASN:OD1  | 3:O1:210:GLY:N    | 2.26                     | 0.64              |
| 20:B2:82:LEU:HD11 | 52:12:126:LYS:HE3 | 1.80                     | 0.64              |
| 49:h2:141:CYS:HA  | 54:g2:162:ARG:HD3 | 1.80                     | 0.64              |
| 56:A3:172:LYS:HB2 | 56:A3:172:LYS:NZ  | 2.12                     | 0.64              |
| 1:A1:358:LYS:HD2  | 1:A1:402:VAL:CG1  | 2.28                     | 0.64              |
| 2:B1:24:LEU:HD12  | 2:B1:24:LEU:N     | 2.04                     | 0.64              |
| 2:B1:95:LYS:HE3   | 9:I1:70:LEU:CD2   | 2.24                     | 0.64              |
| 2:B1:347:ILE:HD12 | 2:B1:347:ILE:N    | 2.13                     | 0.64              |
| 3:C1:338:ILE:N    | 3:C1:338:ILE:CD1  | 2.61                     | 0.64              |
| 2:N1:352:LEU:HG   | 2:N1:352:LEU:O    | 1.96                     | 0.64              |
| 5:Q1:63:SER:O     | 5:Q1:64:ALA:HB2   | 1.98                     | 0.64              |
| 56:A3:84:PRO:HG3  | 56:A3:92:MET:HE3  | 1.80                     | 0.64              |
| 59:D3:24:LEU:H    | 60:E3:34:ASN:HD21 | 1.44                     | 0.64              |
| 1:A1:145:MET:SD   | 1:A1:248:LEU:CD1  | 2.86                     | 0.64              |
| 2:B1:434:PRO:HB3  | 2:B1:438:GLU:HB3  | 1.80                     | 0.64              |
| 3:C1:47:THR:HG21  | 3:C1:83:HIS:CB    | 2.27                     | 0.64              |
| 3:C1:309:THR:HG23 | 3:C1:370:GLY:HA3  | 1.80                     | 0.64              |
| 4:D1:94:PRO:HB2   | 4:D1:95:TYR:CE1   | 2.33                     | 0.64              |
| 10:J1:34:ALA:O    | 10:J1:35:PHE:C    | 2.38                     | 0.64              |
| 1:M1:15:GLN:O     | 1:M1:26:ALA:HA    | 1.97                     | 0.64              |
| 1:M1:199:ALA:HB3  | 1:M1:208:LEU:HD21 | 1.79                     | 0.64              |
| 3:O1:79:ILE:HG12  | 5:Q1:58:PHE:CE1   | 2.33                     | 0.64              |
| 5:Q1:15:ARG:CB    | 5:Q1:16:PRO:HD2   | 2.06                     | 0.64              |
| 6:R1:43:VAL:HG22  | 6:R1:94:LEU:HD21  | 1.80                     | 0.64              |
| 7:S1:34:ILE:HB    | 7:S1:35:PRO:CD    | 2.27                     | 0.64              |
| 19:A2:362:ASP:CG  | 29:K2:17:ARG:HH21 | 2.06                     | 0.64              |
| 1:A1:338:LEU:O    | 1:A1:339:GLN:C    | 2.41                     | 0.64              |
| 2:B1:319:SER:OG   | 2:B1:320:GLY:N    | 2.27                     | 0.64              |
| 3:C1:78:ILE:O     | 3:C1:82:MET:HB2   | 1.98                     | 0.64              |
| 1:M1:408:ARG:NH1  | 11:W1:15:ARG:HG2  | 2.13                     | 0.64              |
| 3:O1:141:TRP:O    | 3:O1:145:VAL:HG23 | 1.98                     | 0.64              |
| 5:Q1:118:ARG:HB3  | 5:Q1:171:ILE:HG23 | 1.80                     | 0.64              |
| 1:A1:385:THR:HG22 | 1:A1:386:TYR:N    | 2.12                     | 0.63              |
| 3:C1:183:PHE:CD1  | 3:O1:183:PHE:CE1  | 2.86                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:F1:96:GLU:OE1   | 6:F1:99:ARG:HD2    | 1.98                     | 0.63              |
| 7:G1:34:ILE:HB    | 7:G1:35:PRO:CD     | 2.21                     | 0.63              |
| 3:O1:119:LEU:HD13 | 3:O1:192:ILE:HG22  | 1.80                     | 0.63              |
| 5:Q1:15:ARG:HH21  | 5:Q1:32:ARG:CG     | 2.08                     | 0.63              |
| 52:12:288:LEU:HA  | 52:12:292:ASN:HD22 | 1.63                     | 0.63              |
| 53:62:578:THR:HA  | 53:62:581:LYS:HE2  | 1.79                     | 0.63              |
| 1:A1:64:PHE:CE2   | 1:A1:88:ALA:HB2    | 2.33                     | 0.63              |
| 1:A1:204:GLU:HG2  | 1:A1:206:ARG:HB3   | 1.80                     | 0.63              |
| 2:B1:109:VAL:HG22 | 2:B1:119:LEU:CD2   | 2.28                     | 0.63              |
| 1:M1:426:GLY:CA   | 1:M1:428:ILE:N     | 2.61                     | 0.63              |
| 3:O1:30:TRP:O     | 3:O1:33:PHE:CD2    | 2.47                     | 0.63              |
| 6:R1:96:GLU:OE1   | 6:R1:99:ARG:HD2    | 1.98                     | 0.63              |
| 19:A2:313:LEU:N   | 38:U2:142:THR:O    | 2.30                     | 0.63              |
| 56:A3:187:SER:CB  | 56:A3:277:MET:HE1  | 2.28                     | 0.63              |
| 2:B1:384:SER:CB   | 9:I1:62:ARG:HG2    | 2.28                     | 0.63              |
| 3:C1:44:GLN:OE1   | 3:C1:83:HIS:ND1    | 2.30                     | 0.63              |
| 1:M1:143:THR:HG23 | 1:M1:143:THR:O     | 1.98                     | 0.63              |
| 1:M1:385:THR:HG22 | 1:M1:386:TYR:N     | 2.13                     | 0.63              |
| 4:P1:50:HIS:HB3   | 4:P1:54:VAL:CG2    | 2.28                     | 0.63              |
| 5:Q1:193:VAL:HG13 | 5:Q1:193:VAL:O     | 1.97                     | 0.63              |
| 7:S1:25:ALA:C     | 7:S1:27:PRO:HD3    | 2.23                     | 0.63              |
| 3:C1:78:ILE:HG21  | 4:D1:204:MET:HE1   | 1.81                     | 0.63              |
| 3:C1:230:LEU:HD12 | 4:D1:219:VAL:HG12  | 1.80                     | 0.63              |
| 1:M1:352:SER:OG   | 1:M1:353:GLU:N     | 2.31                     | 0.63              |
| 3:O1:102:LEU:HB3  | 3:O1:325:PHE:HE1   | 1.62                     | 0.63              |
| 5:Q1:157:TYR:CE2  | 5:Q1:159:PRO:HA    | 2.33                     | 0.63              |
| 10:V1:51:LEU:HD22 | 10:V1:52:TRP:HZ3   | 1.64                     | 0.63              |
| 53:62:138:PHE:HB2 | 53:62:196:TRP:HE1  | 1.62                     | 0.63              |
| 2:B1:338:LYS:HD3  | 2:B1:439:LEU:HD23  | 1.81                     | 0.63              |
| 3:C1:183:PHE:CD1  | 3:C1:183:PHE:O     | 2.52                     | 0.63              |
| 3:C1:346:PRO:HG2  | 7:G1:66:PHE:HD1    | 1.63                     | 0.63              |
| 4:D1:32:VAL:HG21  | 4:D1:186:VAL:HG22  | 1.79                     | 0.63              |
| 1:M1:72:GLY:O     | 1:M1:73:ASN:OD1    | 2.17                     | 0.63              |
| 39:V2:58:ARG:HE   | 52:12:316:PRO:HB3  | 1.63                     | 0.63              |
| 53:62:28:LYS:HE3  | 53:62:31:ASN:HD21  | 1.63                     | 0.63              |
| 56:A3:273:MET:HG3 | 56:A3:319:LYS:HZ1  | 1.63                     | 0.63              |
| 1:A1:308:GLN:O    | 1:A1:308:GLN:CG    | 2.46                     | 0.63              |
| 1:A1:333:ASP:O    | 1:A1:337:VAL:HG23  | 1.98                     | 0.63              |
| 2:B1:59:ASN:CG    | 2:B1:60:SER:H      | 2.07                     | 0.63              |
| 3:C1:311:LYS:O    | 6:F1:38:HIS:HB2    | 1.98                     | 0.63              |
| 4:D1:82:MET:CE    | 4:D1:86:LYS:HZ2    | 2.11                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D1:138:PRO:O     | 4:D1:139:THR:C    | 2.40                     | 0.63              |
| 3:O1:137:GLN:OE1   | 3:O1:259:ALA:HA   | 1.99                     | 0.63              |
| 4:P1:229:VAL:HG12  | 4:P1:233:ARG:HE   | 1.63                     | 0.63              |
| 2:B1:341:TYR:HE2   | 2:B1:345:LYS:HE3  | 1.61                     | 0.63              |
| 10:J1:3:PRO:HG2    | 10:J1:8:ARG:HG2   | 1.81                     | 0.63              |
| 1:M1:155:ALA:HA    | 1:M1:164:ALA:HB1  | 1.80                     | 0.63              |
| 1:M1:350:THR:HB    | 1:M1:353:GLU:CG   | 2.28                     | 0.63              |
| 1:M1:404:ALA:O     | 1:M1:408:ARG:HG3  | 1.98                     | 0.63              |
| 2:N1:257:LEU:HD13  | 2:N1:424:MET:HE2  | 1.80                     | 0.63              |
| 4:P1:75:ASN:ND2    | 4:P1:80:MET:O     | 2.32                     | 0.63              |
| 5:Q1:76:ILE:HG22   | 5:Q1:194:ILE:HG12 | 1.79                     | 0.63              |
| 19:A2:314:LEU:HD22 | 38:U2:140:PRO:HD2 | 1.77                     | 0.63              |
| 52:12:75:PRO:N     | 52:12:223:PHE:CZ  | 2.64                     | 0.63              |
| 4:D1:10:TYR:O      | 4:D1:12:TRP:CD1   | 2.51                     | 0.63              |
| 6:F1:75:LEU:O      | 6:F1:80:TRP:NE1   | 2.30                     | 0.63              |
| 3:O1:90:PHE:HE1    | 3:O1:123:VAL:HG21 | 1.60                     | 0.63              |
| 3:O1:115:ILE:CG2   | 3:O1:196:HIS:HB2  | 2.27                     | 0.63              |
| 3:O1:153:ILE:HG23  | 3:O1:154:PRO:HD2  | 1.79                     | 0.63              |
| 3:C1:15:ASN:ND2    | 3:C1:18:PHE:CE1   | 2.67                     | 0.63              |
| 3:C1:296:PHE:CD1   | 3:C1:359:PHE:HE1  | 2.17                     | 0.63              |
| 7:G1:71:ARG:HH21   | 8:H1:60:ASP:CG    | 2.07                     | 0.63              |
| 1:M1:151:ASN:ND2   | 5:Q1:2:HIS:NE2    | 2.46                     | 0.63              |
| 3:O1:28:SER:HB3    | 3:O1:30:TRP:HD1   | 1.63                     | 0.63              |
| 3:O1:33:PHE:CE1    | 3:O1:96:MET:HG3   | 2.34                     | 0.63              |
| 3:O1:132:VAL:HA    | 3:O1:139:SER:HB3  | 1.81                     | 0.63              |
| 19:A2:302:LEU:N    | 38:U2:137:TRP:HB2 | 2.13                     | 0.63              |
| 67:L3:45:LEU:HD21  | 68:M3:40:TYR:HA   | 1.78                     | 0.63              |
| 1:A1:38:GLY:HA3    | 1:A1:40:TRP:HZ3   | 1.62                     | 0.62              |
| 3:C1:119:LEU:HD13  | 3:C1:192:ILE:HG22 | 1.80                     | 0.62              |
| 1:M1:86:LEU:HB3    | 2:N1:285:VAL:HG22 | 1.81                     | 0.62              |
| 2:N1:83:PHE:CE2    | 2:N1:87:ARG:HG3   | 2.34                     | 0.62              |
| 3:O1:207:ASN:HB2   | 3:O1:208:PRO:HD2  | 1.80                     | 0.62              |
| 49:h2:141:CYS:HB2  | 49:h2:144:PRO:HG3 | 1.81                     | 0.62              |
| 60:E3:82:TYR:HB3   | 60:E3:83:PRO:HD3  | 1.81                     | 0.62              |
| 1:A1:370:ASP:OD1   | 2:B1:375:SER:HB3  | 1.99                     | 0.62              |
| 2:B1:352:LEU:HB3   | 2:B1:411:ILE:CD1  | 2.29                     | 0.62              |
| 1:M1:45:SER:CB     | 1:M1:167:VAL:HG22 | 2.29                     | 0.62              |
| 4:P1:50:HIS:O      | 4:P1:51:LEU:C     | 2.40                     | 0.62              |
| 4:P1:62:LYS:O      | 4:P1:66:GLU:HG3   | 1.99                     | 0.62              |
| 1:A1:297:ILE:HG22  | 1:A1:303:LEU:HD12 | 1.79                     | 0.62              |
| 2:B1:111:CYS:CB    | 2:B1:119:LEU:HD22 | 2.28                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C1:116:GLY:HA3  | 69:C1:402:HEM:C3C  | 2.34                     | 0.62              |
| 3:O1:160:LEU:HD11 | 3:O1:164:ILE:HD11  | 1.80                     | 0.62              |
| 5:Q1:153:PHE:CE1  | 5:Q1:173:LYS:HG3   | 2.34                     | 0.62              |
| 59:D3:16:TYR:CE1  | 59:D3:25:PRO:HG3   | 2.34                     | 0.62              |
| 63:H3:57:ARG:HB3  | 63:H3:57:ARG:HH11  | 1.64                     | 0.62              |
| 1:A1:351:GLU:OE2  | 1:A1:404:ALA:HB3   | 2.00                     | 0.62              |
| 1:A1:351:GLU:O    | 1:A1:352:SER:C     | 2.42                     | 0.62              |
| 1:A1:403:ASP:OD1  | 1:A1:404:ALA:N     | 2.33                     | 0.62              |
| 2:B1:47:ILE:HG22  | 2:B1:48:GLY:N      | 2.15                     | 0.62              |
| 2:B1:156:GLN:NE2  | 9:I1:56:ARG:HD3    | 2.14                     | 0.62              |
| 3:C1:119:LEU:HD13 | 3:C1:192:ILE:CG2   | 2.29                     | 0.62              |
| 3:C1:207:ASN:OD1  | 3:C1:210:GLY:N     | 2.32                     | 0.62              |
| 4:D1:50:HIS:HB3   | 4:D1:54:VAL:CG2    | 2.29                     | 0.62              |
| 1:M1:309:THR:HA   | 1:M1:322:ALA:HA    | 1.81                     | 0.62              |
| 2:N1:154:ASN:O    | 2:N1:155:PRO:C     | 2.43                     | 0.62              |
| 8:T1:34:ARG:O     | 8:T1:38:GLU:HG2    | 1.99                     | 0.62              |
| 19:A2:129:PRO:CG  | 27:I2:114:TYR:HE1  | 2.12                     | 0.62              |
| 34:Q2:50:GLU:HB3  | 34:Q2:138:PRO:HG3  | 1.80                     | 0.62              |
| 56:A3:92:MET:HE2  | 56:A3:167:THR:HG21 | 1.82                     | 0.62              |
| 57:B3:122:MET:HB2 | 57:B3:208:PRO:HD2  | 1.81                     | 0.62              |
| 2:B1:341:TYR:CE2  | 2:B1:345:LYS:HE3   | 2.34                     | 0.62              |
| 3:C1:27:ILE:O     | 3:C1:27:ILE:CG2    | 2.46                     | 0.62              |
| 2:N1:37:SER:OG    | 2:N1:213:HIS:HB2   | 2.00                     | 0.62              |
| 2:N1:56:ARG:NH2   | 2:N1:172:LEU:HD21  | 2.14                     | 0.62              |
| 2:N1:95:LYS:CE    | 9:U1:70:LEU:HD22   | 2.29                     | 0.62              |
| 4:P1:127:VAL:HG12 | 4:P1:187:CYS:SG    | 2.39                     | 0.62              |
| 5:Q1:76:ILE:HG23  | 5:Q1:194:ILE:CG1   | 2.29                     | 0.62              |
| 5:Q1:78:LEU:HD23  | 5:Q1:79:SER:H      | 1.64                     | 0.62              |
| 17:82:52:ARG:HH21 | 17:82:132:ARG:HG3  | 1.63                     | 0.62              |
| 1:A1:43:ALA:CB    | 1:A1:189:HIS:HB3   | 2.30                     | 0.62              |
| 1:A1:92:ARG:HD2   | 1:A1:163:LEU:CD1   | 2.29                     | 0.62              |
| 1:A1:158:PHE:CB   | 1:A1:164:ALA:HB2   | 2.29                     | 0.62              |
| 4:D1:72:ASP:O     | 4:D1:73:GLY:O      | 2.18                     | 0.62              |
| 6:F1:106:GLU:HA   | 6:F1:109:LYS:HZ3   | 1.63                     | 0.62              |
| 8:H1:25:GLU:HA    | 8:H1:30:CYS:SG     | 2.39                     | 0.62              |
| 2:N1:203:ARG:NE   | 2:N1:230:LEU:HD23  | 2.15                     | 0.62              |
| 2:N1:255:ALA:HB2  | 2:N1:426:ALA:HB2   | 1.81                     | 0.62              |
| 3:O1:8:HIS:CB     | 3:O1:9:PRO:HD3     | 2.29                     | 0.62              |
| 4:P1:3:LEU:HD11   | 7:S1:71:ARG:HB2    | 1.81                     | 0.62              |
| 9:U1:53:GLU:O     | 9:U1:55:LEU:HG     | 2.00                     | 0.62              |
| 1:A1:6:GLN:O      | 1:A1:7:ALA:C       | 2.41                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:91:THR:CG2    | 1:A1:92:ARG:N      | 2.62                     | 0.62              |
| 1:A1:240:GLN:HG3   | 1:A1:422:VAL:O     | 1.98                     | 0.62              |
| 1:A1:417:ASP:OD1   | 1:A1:417:ASP:O     | 2.17                     | 0.62              |
| 2:B1:42:ALA:CB     | 2:B1:43:PRO:HD2    | 2.28                     | 0.62              |
| 2:B1:187:THR:O     | 2:B1:190:GLU:HB2   | 1.99                     | 0.62              |
| 3:C1:106:SER:HB3   | 69:C1:402:HEM:HBD2 | 1.81                     | 0.62              |
| 3:O1:115:ILE:HG21  | 3:O1:196:HIS:HB2   | 1.81                     | 0.62              |
| 10:V1:51:LEU:HB3   | 10:V1:52:TRP:CE3   | 2.35                     | 0.62              |
| 11:W1:26:ALA:O     | 11:W1:30:VAL:HG23  | 1.99                     | 0.62              |
| 19:A2:423:LEU:HD12 | 25:G2:169:ARG:O    | 1.98                     | 0.62              |
| 27:I2:96:HIS:HB2   | 27:I2:114:TYR:HB3  | 1.81                     | 0.62              |
| 1:A1:32:GLN:HG3    | 1:A1:33:PRO:HD2    | 1.80                     | 0.62              |
| 1:A1:61:HIS:NE2    | 1:A1:134:ILE:CD1   | 2.62                     | 0.62              |
| 1:A1:408:ARG:NH1   | 11:K1:15:ARG:NE    | 2.45                     | 0.62              |
| 2:B1:58:GLU:OE1    | 2:B1:63:LEU:HA     | 2.00                     | 0.62              |
| 2:B1:156:GLN:HE22  | 9:I1:56:ARG:HD3    | 1.65                     | 0.62              |
| 2:B1:163:LEU:HD22  | 2:B1:256:ALA:CB    | 2.29                     | 0.62              |
| 2:B1:247:GLN:NE2   | 2:B1:429:ASN:HA    | 2.14                     | 0.62              |
| 5:Q1:103:LYS:HA    | 5:Q1:106:ILE:HD12  | 1.82                     | 0.62              |
| 2:B1:58:GLU:HB2    | 2:B1:63:LEU:HD23   | 1.82                     | 0.62              |
| 2:B1:101:THR:OG1   | 2:B1:102:ARG:N     | 2.32                     | 0.62              |
| 3:C1:329:VAL:HA    | 3:C1:332:LEU:HD12  | 1.80                     | 0.62              |
| 4:D1:57:THR:HG22   | 4:D1:58:GLU:H      | 1.65                     | 0.62              |
| 1:M1:53:ASN:OD1    | 1:M1:170:PRO:HD3   | 1.99                     | 0.62              |
| 1:M1:134:ILE:HG21  | 1:M1:174:VAL:HG21  | 1.81                     | 0.62              |
| 1:M1:144:SER:O     | 1:M1:148:VAL:HG23  | 1.99                     | 0.62              |
| 2:N1:195:VAL:HG13  | 2:N1:199:PHE:CD2   | 2.34                     | 0.62              |
| 2:N1:352:LEU:HB3   | 2:N1:411:ILE:CD1   | 2.29                     | 0.62              |
| 4:P1:120:ARG:HG2   | 4:P1:120:ARG:HH11  | 1.62                     | 0.62              |
| 4:P1:231:LYS:HD2   | 6:R1:71:ARG:HG2    | 1.81                     | 0.62              |
| 5:Q1:187:PHE:CE2   | 5:Q1:193:VAL:HB    | 2.34                     | 0.62              |
| 17:82:384:PRO:HD3  | 19:A2:76:ARG:HB2   | 1.82                     | 0.62              |
| 19:A2:111:LYS:HE2  | 33:P2:53:TYR:CE2   | 2.35                     | 0.62              |
| 19:A2:313:LEU:CG   | 38:U2:142:THR:CB   | 2.78                     | 0.62              |
| 2:B1:209:LEU:CD2   | 2:B1:375:SER:HB2   | 2.30                     | 0.62              |
| 2:B1:303:VAL:HG12  | 2:B1:304:HIS:N     | 2.14                     | 0.62              |
| 3:C1:25:SER:HA     | 3:C1:218:ILE:CD1   | 2.29                     | 0.62              |
| 3:C1:79:ILE:HG12   | 5:E1:58:PHE:CE1    | 2.35                     | 0.62              |
| 4:D1:82:MET:HE2    | 4:D1:86:LYS:HZ2    | 1.64                     | 0.62              |
| 1:M1:162:PRO:O     | 1:M1:165:GLN:HG2   | 1.99                     | 0.62              |
| 3:O1:7:SER:HA      | 3:O1:13:ILE:HG12   | 1.81                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:52:ALA:HB2    | 69:O1:401:HEM:HMD1 | 1.81                     | 0.62              |
| 4:P1:79:GLU:OE1    | 4:P1:82:MET:HG3    | 1.98                     | 0.62              |
| 4:P1:176:PRO:HB2   | 4:P1:181:GLN:NE2   | 2.14                     | 0.62              |
| 6:R1:73:GLN:HE21   | 7:S1:32:LYS:CE     | 2.12                     | 0.62              |
| 19:A2:140:GLN:HG3  | 20:B2:379:ILE:HG23 | 1.81                     | 0.62              |
| 20:B2:82:LEU:HD11  | 52:12:126:LYS:CD   | 2.30                     | 0.62              |
| 1:A1:395:TRP:O     | 1:A1:396:GLU:C     | 2.43                     | 0.61              |
| 1:A1:433:ASP:HB2   | 3:C1:219:PRO:HG2   | 1.82                     | 0.61              |
| 3:C1:10:LEU:HD12   | 3:C1:13:ILE:CD1    | 2.28                     | 0.61              |
| 2:N1:129:ALA:N     | 2:N1:130:PRO:HD3   | 2.14                     | 0.61              |
| 56:A3:128:VAL:HG22 | 56:A3:128:VAL:O    | 1.99                     | 0.61              |
| 1:A1:151:ASN:O     | 1:A1:152:TYR:C     | 2.43                     | 0.61              |
| 1:A1:336:PHE:HE2   | 1:A1:446:PHE:HD2   | 1.47                     | 0.61              |
| 2:B1:111:CYS:HB3   | 2:B1:119:LEU:CD2   | 2.29                     | 0.61              |
| 3:C1:207:ASN:ND2   | 3:C1:209:THR:OG1   | 2.32                     | 0.61              |
| 3:C1:313:ARG:HB3   | 6:F1:38:HIS:CD2    | 2.35                     | 0.61              |
| 10:J1:51:LEU:HB3   | 10:J1:52:TRP:CZ3   | 2.36                     | 0.61              |
| 1:M1:373:THR:HB    | 1:M1:374:PRO:HD3   | 1.81                     | 0.61              |
| 3:O1:304:ILE:N     | 3:O1:305:PRO:HD2   | 2.14                     | 0.61              |
| 18:92:130:TYR:HA   | 18:92:189:ASN:HD21 | 1.65                     | 0.61              |
| 19:A2:34:VAL:HG22  | 19:A2:99:GLY:HA2   | 1.82                     | 0.61              |
| 19:A2:667:GLN:HE22 | 29:K2:38:GLU:CD    | 2.07                     | 0.61              |
| 57:B3:16:ILE:HD12  | 57:B3:17:MET:N     | 2.15                     | 0.61              |
| 2:B1:47:ILE:HD12   | 2:B1:120:MET:SD    | 2.39                     | 0.61              |
| 2:B1:90:GLU:O      | 2:B1:91:ALA:C      | 2.44                     | 0.61              |
| 2:B1:169:ARG:CZ    | 2:N1:438:GLU:OE2   | 2.47                     | 0.61              |
| 3:O1:8:HIS:CB      | 3:O1:9:PRO:CD      | 2.78                     | 0.61              |
| 4:P1:68:VAL:HG12   | 4:P1:92:PRO:HG2    | 1.82                     | 0.61              |
| 4:P1:83:ARG:CB     | 4:P1:84:PRO:CD     | 2.63                     | 0.61              |
| 4:P1:138:PRO:HG2   | 8:T1:55:THR:CB     | 2.30                     | 0.61              |
| 10:V1:55:ILE:HG23  | 10:V1:58:LYS:HE2   | 1.82                     | 0.61              |
| 22:D2:99:MET:HG2   | 22:D2:106:MET:HB2  | 1.83                     | 0.61              |
| 61:F3:13:ALA:O     | 61:F3:18:ARG:HD2   | 2.00                     | 0.61              |
| 1:A1:5:ALA:O       | 1:A1:8:LEU:HB2     | 2.00                     | 0.61              |
| 1:A1:428:ILE:HG21  | 1:A1:431:LEU:HD22  | 1.83                     | 0.61              |
| 2:B1:123:LEU:O     | 2:B1:127:THR:HG22  | 2.00                     | 0.61              |
| 2:B1:162:ASN:ND2   | 2:B1:244:ILE:CG2   | 2.61                     | 0.61              |
| 3:C1:52:ALA:HB2    | 69:C1:401:HEM:HMD2 | 1.83                     | 0.61              |
| 3:C1:153:ILE:HG23  | 3:C1:154:PRO:HD2   | 1.82                     | 0.61              |
| 10:J1:29:LEU:HD13  | 11:K1:34:TRP:HB3   | 1.81                     | 0.61              |
| 5:Q1:141:HIS:NE2   | 5:Q1:175:PRO:HB2   | 2.15                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:S1:54:ALA:O      | 7:S1:58:VAL:HG23   | 2.01                     | 0.61              |
| 17:82:419:ILE:HD11 | 19:A2:119:PHE:HE2  | 1.65                     | 0.61              |
| 51:j2:119:VAL:H    | 54:g2:147:GLY:H    | 1.47                     | 0.61              |
| 58:C3:154:GLY:HA2  | 61:F3:6:VAL:CG2    | 2.30                     | 0.61              |
| 65:J3:3:ASN:HD22   | 65:J3:3:ASN:C      | 2.08                     | 0.61              |
| 3:C1:372:ILE:O     | 3:C1:375:LYS:N     | 2.32                     | 0.61              |
| 1:M1:403:ASP:OD1   | 1:M1:404:ALA:N     | 2.33                     | 0.61              |
| 2:N1:354:ASN:N     | 2:N1:355:PRO:HD2   | 2.16                     | 0.61              |
| 3:O1:126:THR:HG21  | 69:O1:401:HEM:C3B  | 2.36                     | 0.61              |
| 8:T1:15:ASP:HB2    | 8:T1:16:PRO:HD3    | 1.83                     | 0.61              |
| 19:A2:129:PRO:HG2  | 27:I2:114:TYR:HE1  | 1.65                     | 0.61              |
| 19:A2:313:LEU:CD2  | 38:U2:142:THR:HA   | 2.31                     | 0.61              |
| 20:B2:95:LEU:O     | 20:B2:95:LEU:HD23  | 2.01                     | 0.61              |
| 3:C1:267:HIS:NE2   | 3:C1:269:LYS:HD3   | 2.15                     | 0.61              |
| 4:D1:204:MET:O     | 4:D1:205:GLY:C     | 2.42                     | 0.61              |
| 9:I1:62:ARG:HB3    | 9:I1:63:PRO:HD3    | 1.83                     | 0.61              |
| 1:M1:37:VAL:HG13   | 1:M1:199:ALA:HB2   | 1.82                     | 0.61              |
| 1:M1:358:LYS:HE3   | 1:M1:402:VAL:HB    | 1.82                     | 0.61              |
| 3:O1:171:ASP:O     | 3:O1:172:LYS:C     | 2.44                     | 0.61              |
| 4:P1:27:ARG:NH2    | 4:P1:60:GLU:OE2    | 2.34                     | 0.61              |
| 4:P1:27:ARG:HH11   | 10:V1:58:LYS:NZ    | 1.98                     | 0.61              |
| 7:S1:73:ASN:HD22   | 8:T1:56:GLU:CD     | 2.08                     | 0.61              |
| 19:A2:273:ILE:HD11 | 19:A2:291:ARG:HA   | 1.83                     | 0.61              |
| 40:M2:70:LEU:HD13  | 40:M2:76:ILE:HG12  | 1.82                     | 0.61              |
| 1:A1:436:ARG:HE    | 3:C1:222:PRO:CG    | 2.12                     | 0.61              |
| 2:B1:86:THR:HG23   | 9:I1:71:ASN:HD21   | 1.66                     | 0.61              |
| 3:C1:146:ILE:O     | 3:C1:149:LEU:HB3   | 2.00                     | 0.61              |
| 8:H1:40:CYS:HB2    | 8:H1:57:GLU:HG2    | 1.83                     | 0.61              |
| 2:N1:412:ASN:O     | 2:N1:415:LYS:HB2   | 2.01                     | 0.61              |
| 14:42:294:MET:SD   | 14:42:319:HIS:NE2  | 2.70                     | 0.61              |
| 52:12:75:PRO:HG3   | 52:12:223:PHE:CE2  | 2.32                     | 0.61              |
| 56:A3:92:MET:CE    | 56:A3:167:THR:HG21 | 2.31                     | 0.61              |
| 58:C3:6:HIS:HD2    | 58:C3:8:TYR:H      | 1.49                     | 0.61              |
| 2:B1:140:LEU:HD12  | 2:B1:143:GLN:HB3   | 1.83                     | 0.61              |
| 3:O1:244:LEU:HD23  | 4:P1:205:GLY:HA2   | 1.83                     | 0.61              |
| 4:P1:13:SER:O      | 4:P1:19:SER:HB3    | 1.99                     | 0.61              |
| 19:A2:67:GLU:HA    | 25:G2:158:LYS:HE2  | 1.81                     | 0.61              |
| 47:d2:77:PHE:HA    | 53:62:471:ASN:HD21 | 1.65                     | 0.61              |
| 56:A3:11:ASN:HD21  | 56:A3:13:LYS:HB2   | 1.64                     | 0.61              |
| 2:B1:435:PHE:HB2   | 2:B1:438:GLU:OE1   | 2.00                     | 0.61              |
| 3:C1:315:MET:HA    | 3:C1:318:ARG:HG3   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M1:354:VAL:CG1  | 1:M1:407:VAL:HG21 | 2.31                     | 0.61              |
| 4:P1:11:PRO:O     | 8:T1:74:PHE:CZ    | 2.54                     | 0.61              |
| 20:B2:87:GLN:HA   | 20:B2:87:GLN:OE1  | 2.01                     | 0.61              |
| 58:C3:148:HIS:O   | 58:C3:152:MET:HG3 | 2.01                     | 0.61              |
| 68:M3:13:LYS:HD3  | 68:M3:13:LYS:H    | 1.65                     | 0.61              |
| 1:A1:86:LEU:HD13  | 1:A1:99:ILE:CG1   | 2.31                     | 0.61              |
| 1:A1:244:ARG:CZ   | 7:G1:10:VAL:HB    | 2.31                     | 0.61              |
| 2:B1:59:ASN:OD1   | 2:B1:60:SER:N     | 2.32                     | 0.61              |
| 2:B1:434:PRO:HB2  | 2:B1:439:LEU:HD11 | 1.81                     | 0.61              |
| 3:C1:22:PRO:CG    | 7:G1:3:GLN:HB3    | 2.31                     | 0.61              |
| 4:D1:10:TYR:CE1   | 8:H1:73:LEU:CD2   | 2.84                     | 0.61              |
| 5:E1:29:SER:HA    | 5:E1:32:ARG:HD3   | 1.81                     | 0.61              |
| 1:M1:4:TYR:CE2    | 1:M1:396:GLU:HG3  | 2.36                     | 0.61              |
| 1:M1:366:VAL:HG12 | 1:M1:367:SER:N    | 2.16                     | 0.61              |
| 3:O1:129:MET:CG   | 3:O1:178:PHE:HD1  | 2.14                     | 0.61              |
| 5:Q1:13:TYR:O     | 7:S1:23:GLN:HB3   | 2.01                     | 0.61              |
| 63:H3:39:CYS:HG   | 63:H3:53:CYS:CB   | 2.09                     | 0.61              |
| 1:A1:5:ALA:O      | 1:A1:6:GLN:C      | 2.43                     | 0.60              |
| 1:A1:80:GLU:O     | 1:A1:82:MET:N     | 2.34                     | 0.60              |
| 2:B1:337:ILE:CG2  | 2:B1:434:PRO:HG2  | 2.31                     | 0.60              |
| 3:C1:163:TRP:O    | 3:C1:177:ARG:NH1  | 2.32                     | 0.60              |
| 7:G1:68:LYS:O     | 7:G1:72:LYS:N     | 2.34                     | 0.60              |
| 1:M1:91:THR:HG23  | 1:M1:92:ARG:N     | 2.16                     | 0.60              |
| 4:P1:237:TYR:CD2  | 4:P1:239:PRO:HD3  | 2.36                     | 0.60              |
| 25:G2:75:ARG:NH2  | 25:G2:119:ASP:OD1 | 2.34                     | 0.60              |
| 1:A1:41:ILE:CG1   | 1:A1:195:MET:HE3  | 2.22                     | 0.60              |
| 1:A1:236:PHE:HD2  | 1:A1:258:GLU:CG   | 2.12                     | 0.60              |
| 2:B1:155:PRO:O    | 2:B1:156:GLN:C    | 2.43                     | 0.60              |
| 7:G1:25:ALA:C     | 7:G1:27:PRO:HD3   | 2.26                     | 0.60              |
| 5:Q1:188:THR:OG1  | 5:Q1:189:SER:N    | 2.33                     | 0.60              |
| 19:A2:313:LEU:HG  | 38:U2:142:THR:CA  | 2.31                     | 0.60              |
| 20:B2:97:LEU:HD12 | 20:B2:97:LEU:N    | 2.01                     | 0.60              |
| 46:c2:25:ASP:OD2  | 48:f2:125:TRP:NE1 | 2.35                     | 0.60              |
| 1:A1:182:LEU:O    | 1:A1:186:LEU:HD12 | 2.01                     | 0.60              |
| 1:A1:413:LYS:HB2  | 1:A1:414:TYR:CD2  | 2.37                     | 0.60              |
| 2:B1:60:SER:CB    | 2:N1:429:ASN:ND2  | 2.53                     | 0.60              |
| 2:B1:196:GLN:HG2  | 2:B1:197:ASN:OD1  | 2.01                     | 0.60              |
| 2:B1:256:ALA:O    | 2:B1:424:MET:HG3  | 2.01                     | 0.60              |
| 2:B1:299:VAL:O    | 2:B1:303:VAL:HG23 | 2.01                     | 0.60              |
| 3:C1:18:PHE:O     | 3:C1:220:PHE:HD2  | 1.84                     | 0.60              |
| 4:D1:165:TYR:CE1  | 4:D1:168:VAL:HG22 | 2.34                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F1:106:GLU:HA   | 6:F1:109:LYS:NZ   | 2.16                     | 0.60              |
| 7:G1:71:ARG:O     | 8:H1:56:GLU:OE2   | 2.20                     | 0.60              |
| 1:M1:365:LEU:O    | 1:M1:365:LEU:HG   | 1.99                     | 0.60              |
| 57:B3:226:MET:O   | 57:B3:227:LEU:HB2 | 2.02                     | 0.60              |
| 1:A1:327:ASP:OD1  | 1:A1:328:HIS:N    | 2.32                     | 0.60              |
| 3:C1:26:ASN:O     | 3:C1:27:ILE:HG13  | 2.01                     | 0.60              |
| 3:C1:218:ILE:HG22 | 3:C1:223:TYR:CD2  | 2.35                     | 0.60              |
| 3:C1:296:PHE:O    | 3:C1:300:ILE:HB   | 2.01                     | 0.60              |
| 4:D1:27:ARG:NH2   | 4:D1:60:GLU:OE2   | 2.33                     | 0.60              |
| 6:F1:28:LYS:HD3   | 6:F1:74:ILE:HD11  | 1.84                     | 0.60              |
| 9:I1:58:GLN:O     | 9:I1:59:ALA:HB2   | 2.01                     | 0.60              |
| 9:I1:58:GLN:HA    | 9:I1:78:TYR:CD2   | 2.36                     | 0.60              |
| 9:I1:62:ARG:N     | 9:I1:63:PRO:HD2   | 2.17                     | 0.60              |
| 2:N1:56:ARG:NE    | 2:N1:103:GLU:OE1  | 2.19                     | 0.60              |
| 19:A2:302:LEU:HB3 | 38:U2:137:TRP:CG  | 2.35                     | 0.60              |
| 1:A1:154:HIS:O    | 1:A1:158:PHE:HB2  | 2.00                     | 0.60              |
| 1:A1:338:LEU:O    | 1:A1:341:GLN:N    | 2.35                     | 0.60              |
| 3:C1:240:MET:CA   | 3:C1:243:VAL:HG12 | 2.28                     | 0.60              |
| 4:D1:165:TYR:CE2  | 4:D1:168:VAL:HG22 | 2.37                     | 0.60              |
| 8:H1:73:LEU:HD21  | 8:H1:74:PHE:CD1   | 2.35                     | 0.60              |
| 1:M1:39:VAL:HG11  | 1:M1:117:VAL:HG21 | 1.81                     | 0.60              |
| 1:M1:312:ILE:HB   | 1:M1:319:LEU:HB2  | 1.83                     | 0.60              |
| 2:N1:34:VAL:HG11  | 2:N1:386:ALA:CB   | 2.32                     | 0.60              |
| 3:O1:206:ASN:CB   | 3:O1:313:ARG:NH2  | 2.55                     | 0.60              |
| 3:O1:296:PHE:CD1  | 3:O1:359:PHE:HE1  | 2.19                     | 0.60              |
| 3:O1:331:ASP:O    | 3:O1:334:THR:HB   | 2.00                     | 0.60              |
| 4:P1:214:LEU:O    | 4:P1:218:LEU:HG   | 2.01                     | 0.60              |
| 9:U1:62:ARG:N     | 9:U1:63:PRO:HD2   | 2.15                     | 0.60              |
| 20:B2:443:MET:SD  | 52:12:281:ARG:NH1 | 2.75                     | 0.60              |
| 53:62:209:SER:OG  | 53:62:270:ASN:ND2 | 2.34                     | 0.60              |
| 1:A1:280:TYR:O    | 1:A1:306:SER:HA   | 2.00                     | 0.60              |
| 1:A1:394:GLU:O    | 1:A1:395:TRP:C    | 2.44                     | 0.60              |
| 2:B1:200:THR:HG22 | 2:B1:203:ARG:CD   | 2.25                     | 0.60              |
| 3:C1:72:ASP:OD1   | 4:D1:49:ARG:NH1   | 2.28                     | 0.60              |
| 4:D1:57:THR:HG22  | 4:D1:58:GLU:N     | 2.17                     | 0.60              |
| 1:M1:55:ALA:O     | 1:M1:56:GLY:C     | 2.43                     | 0.60              |
| 2:N1:362:ASN:HA   | 2:N1:365:LYS:HD3  | 1.83                     | 0.60              |
| 2:N1:385:GLN:HG2  | 9:U1:62:ARG:NH1   | 2.13                     | 0.60              |
| 3:O1:275:LEU:O    | 3:O1:276:PHE:C    | 2.45                     | 0.60              |
| 4:P1:32:VAL:HG11  | 4:P1:186:VAL:CG2  | 2.31                     | 0.60              |
| 5:Q1:29:SER:HA    | 5:Q1:32:ARG:HD3   | 1.83                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:R1:73:GLN:HG2    | 7:S1:36:ASN:HD21  | 1.65                     | 0.60              |
| 21:C2:215:ASP:OD2  | 35:R2:75:ARG:NH2  | 2.34                     | 0.60              |
| 57:B3:59:GLN:HA    | 57:B3:62:GLU:HB2  | 1.83                     | 0.60              |
| 61:F3:62:CYS:SG    | 61:F3:84:SER:OG   | 2.60                     | 0.60              |
| 1:A1:373:THR:HB    | 1:A1:374:PRO:HD3  | 1.84                     | 0.60              |
| 2:B1:98:VAL:HG22   | 2:B1:107:TYR:CD2  | 2.37                     | 0.60              |
| 3:C1:301:LEU:O     | 3:C1:304:ILE:HD12 | 2.02                     | 0.60              |
| 1:M1:64:PHE:CE2    | 1:M1:88:ALA:HB2   | 2.36                     | 0.60              |
| 2:N1:255:ALA:HA    | 2:N1:425:ALA:O    | 2.01                     | 0.60              |
| 2:N1:352:LEU:HD21  | 2:N1:357:VAL:HG23 | 1.82                     | 0.60              |
| 3:O1:196:HIS:HE1   | 69:O1:402:HEM:C1D | 2.19                     | 0.60              |
| 4:P1:42:SER:O      | 4:P1:112:ASP:OD1  | 2.20                     | 0.60              |
| 10:V1:13:LEU:O     | 10:V1:19:THR:OG1  | 2.17                     | 0.60              |
| 20:B2:171:ARG:HH21 | 20:B2:231:GLY:HA2 | 1.66                     | 0.60              |
| 2:B1:217:LYS:O     | 2:B1:218:GLN:C    | 2.45                     | 0.60              |
| 4:D1:30:PHE:HD1    | 4:D1:189:PHE:CE1  | 2.19                     | 0.60              |
| 6:F1:96:GLU:OE2    | 6:F1:99:ARG:NH1   | 2.34                     | 0.60              |
| 5:Q1:97:PHE:CE1    | 5:Q1:137:GLY:HA3  | 2.37                     | 0.60              |
| 19:A2:75:CYS:SG    | 19:A2:76:ARG:N    | 2.75                     | 0.60              |
| 19:A2:143:SER:O    | 20:B2:380:HIS:NE2 | 2.35                     | 0.60              |
| 36:S2:219:SER:HA   | 36:S2:222:LEU:HB2 | 1.83                     | 0.60              |
| 45:b2:134:GLU:HA   | 45:b2:137:MET:HB2 | 1.82                     | 0.60              |
| 4:D1:23:HIS:CD2    | 10:J1:51:LEU:HA   | 2.37                     | 0.60              |
| 1:M1:146:ARG:NH2   | 1:M1:308:GLN:HE22 | 2.00                     | 0.60              |
| 3:O1:4:ILE:O       | 3:O1:4:ILE:HG22   | 2.00                     | 0.60              |
| 3:O1:32:ASN:HD21   | 3:O1:228:ASP:HA   | 1.67                     | 0.60              |
| 5:Q1:164:HIS:H     | 5:Q1:173:LYS:HB2  | 1.67                     | 0.60              |
| 55:e2:36:MET:HA    | 55:e2:77:LYS:HE2  | 1.78                     | 0.60              |
| 58:C3:192:VAL:O    | 58:C3:196:THR:HB  | 2.01                     | 0.60              |
| 1:M1:91:THR:HG22   | 1:M1:94:HIS:H     | 1.67                     | 0.60              |
| 1:M1:363:ASN:CG    | 2:N1:112:LEU:HD23 | 2.27                     | 0.60              |
| 2:N1:269:ALA:O     | 2:N1:272:PHE:N    | 2.35                     | 0.60              |
| 4:P1:134:TYR:HE2   | 4:P1:163:PRO:HG2  | 1.66                     | 0.60              |
| 5:Q1:78:LEU:HD23   | 5:Q1:79:SER:N     | 2.17                     | 0.60              |
| 5:Q1:101:ARG:HD3   | 5:Q1:133:VAL:CG1  | 2.31                     | 0.60              |
| 7:S1:2:ARG:HB2     | 7:S1:6:HIS:CD2    | 2.37                     | 0.60              |
| 68:M3:28:LEU:HB2   | 68:M3:29:PRO:HD3  | 1.84                     | 0.60              |
| 2:B1:258:VAL:CG1   | 2:B1:321:LEU:HB3  | 2.29                     | 0.59              |
| 3:C1:359:PHE:O     | 3:C1:363:LEU:HB2  | 2.02                     | 0.59              |
| 4:D1:28:ARG:HD2    | 4:D1:185:ASP:OD2  | 2.01                     | 0.59              |
| 4:D1:32:VAL:HG11   | 4:D1:182:VAL:HG13 | 1.84                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:92:ILE:O      | 3:O1:96:MET:HG2    | 2.02                     | 0.59              |
| 4:P1:46:VAL:HG12   | 4:P1:47:ALA:O      | 2.02                     | 0.59              |
| 4:P1:72:ASP:O      | 4:P1:73:GLY:O      | 2.20                     | 0.59              |
| 5:Q1:121:GLN:HB3   | 5:Q1:126:ARG:HD3   | 1.83                     | 0.59              |
| 8:T1:37:LEU:HD21   | 8:T1:58:LEU:HA     | 1.84                     | 0.59              |
| 9:U1:78:TYR:HD1    | 9:U1:78:TYR:OXT    | 1.83                     | 0.59              |
| 10:V1:9:LEU:HD12   | 10:V1:13:LEU:CD1   | 2.32                     | 0.59              |
| 10:V1:20:PHE:O     | 10:V1:23:THR:HB    | 2.02                     | 0.59              |
| 18:92:95:ILE:HD11  | 19:A2:210:ILE:HG21 | 1.80                     | 0.59              |
| 31:N2:38:ILE:O     | 31:N2:45:ARG:NH2   | 2.36                     | 0.59              |
| 1:A1:145:MET:HE3   | 1:A1:252:HIS:HE1   | 1.67                     | 0.59              |
| 2:B1:162:ASN:HB3   | 2:B1:244:ILE:HG21  | 1.84                     | 0.59              |
| 2:B1:438:GLU:OE2   | 2:N1:169:ARG:CZ    | 2.51                     | 0.59              |
| 3:C1:312:GLN:HE22  | 3:C1:317:PHE:HB2   | 1.67                     | 0.59              |
| 4:D1:21:LEU:HD11   | 4:D1:192:TRP:HB2   | 1.84                     | 0.59              |
| 4:P1:36:VAL:HG23   | 4:P1:169:LEU:HD11  | 1.84                     | 0.59              |
| 9:U1:62:ARG:HB3    | 9:U1:63:PRO:HD3    | 1.84                     | 0.59              |
| 9:U1:70:LEU:HD12   | 9:U1:71:ASN:N      | 2.16                     | 0.59              |
| 19:A2:130:ILE:HG12 | 27:I2:114:TYR:OH   | 2.02                     | 0.59              |
| 52:12:25:ARG:O     | 52:12:29:GLY:N     | 2.34                     | 0.59              |
| 57:B3:145:PRO:CG   | 57:B3:148:MET:HE2  | 2.33                     | 0.59              |
| 58:C3:119:THR:O    | 62:G3:52:HIS:HE1   | 1.84                     | 0.59              |
| 1:A1:15:GLN:O      | 1:A1:26:ALA:HA     | 2.03                     | 0.59              |
| 1:A1:317:THR:HG22  | 1:A1:318:GLY:H     | 1.67                     | 0.59              |
| 1:A1:350:THR:HB    | 1:A1:353:GLU:HG3   | 1.84                     | 0.59              |
| 3:C1:122:THR:HG23  | 3:C1:185:LEU:HD11  | 1.83                     | 0.59              |
| 4:D1:164:ILE:HD11  | 70:D1:301:HEC:HBB2 | 1.83                     | 0.59              |
| 1:M1:184:GLU:O     | 1:M1:188:ARG:HG3   | 2.02                     | 0.59              |
| 1:M1:426:GLY:HA2   | 1:M1:428:ILE:N     | 2.17                     | 0.59              |
| 2:N1:261:SER:HG    | 2:N1:320:GLY:HA3   | 1.66                     | 0.59              |
| 3:O1:78:ILE:O      | 3:O1:82:MET:HB2    | 2.02                     | 0.59              |
| 5:Q1:118:ARG:NH1   | 5:Q1:171:ILE:CG1   | 2.57                     | 0.59              |
| 7:S1:71:ARG:O      | 8:T1:56:GLU:OE2    | 2.19                     | 0.59              |
| 19:A2:583:ILE:HD13 | 38:U2:137:TRP:CZ3  | 2.37                     | 0.59              |
| 22:D2:114:ARG:HH21 | 22:D2:114:ARG:CG   | 2.13                     | 0.59              |
| 40:M2:37:MET:HG2   | 40:M2:42:LEU:H     | 1.67                     | 0.59              |
| 1:A1:32:GLN:HG2    | 1:A1:33:PRO:CD     | 2.33                     | 0.59              |
| 4:D1:10:TYR:CE1    | 8:H1:73:LEU:HD21   | 2.37                     | 0.59              |
| 7:G1:73:ASN:HD22   | 8:H1:56:GLU:CD     | 2.10                     | 0.59              |
| 1:M1:428:ILE:HG22  | 1:M1:431:LEU:CG    | 2.32                     | 0.59              |
| 3:O1:348:ILE:O     | 3:O1:352:GLN:HG3   | 2.02                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:Q1:45:VAL:HG23   | 10:V1:24:ILE:HA   | 1.83                     | 0.59              |
| 5:Q1:101:ARG:HA    | 5:Q1:105:GLU:OE1  | 2.02                     | 0.59              |
| 8:T1:21:ARG:CB     | 8:T1:65:ARG:HH21  | 2.09                     | 0.59              |
| 11:W1:30:VAL:O     | 11:W1:34:TRP:CG   | 2.56                     | 0.59              |
| 18:92:71:PRO:HA    | 24:F2:102:SER:HB3 | 1.85                     | 0.59              |
| 18:92:149:LEU:HD23 | 18:92:150:GLU:H   | 1.67                     | 0.59              |
| 18:92:236:GLU:OE1  | 18:92:239:LYS:NZ  | 2.35                     | 0.59              |
| 19:A2:302:LEU:CB   | 38:U2:137:TRP:CB  | 2.79                     | 0.59              |
| 60:E3:80:GLU:H     | 60:E3:80:GLU:CD   | 2.10                     | 0.59              |
| 5:E1:33:LYS:HB3    | 7:G1:21:PHE:CE2   | 2.38                     | 0.59              |
| 6:F1:96:GLU:O      | 6:F1:97:VAL:C     | 2.45                     | 0.59              |
| 1:M1:43:ALA:CB     | 1:M1:189:HIS:HB3  | 2.32                     | 0.59              |
| 1:M1:106:LEU:N     | 1:M1:107:PRO:HD2  | 2.18                     | 0.59              |
| 1:M1:408:ARG:NH1   | 11:W1:15:ARG:NE   | 2.47                     | 0.59              |
| 3:O1:242:LEU:HD21  | 3:O1:250:LEU:HD22 | 1.83                     | 0.59              |
| 5:Q1:118:ARG:HH22  | 5:Q1:173:LYS:HA   | 1.66                     | 0.59              |
| 7:S1:25:ALA:O      | 7:S1:27:PRO:HD3   | 2.02                     | 0.59              |
| 52:12:126:LYS:HD3  | 52:12:126:LYS:C   | 2.22                     | 0.59              |
| 57:B3:179:LEU:HD21 | 63:H3:65:PRO:HD3  | 1.85                     | 0.59              |
| 63:H3:57:ARG:HG3   | 63:H3:60:TYR:CE2  | 2.38                     | 0.59              |
| 67:L3:46:LYS:O     | 67:L3:47:LYS:HB2  | 2.02                     | 0.59              |
| 1:A1:11:VAL:HG13   | 1:A1:12:PRO:HD2   | 1.84                     | 0.59              |
| 1:A1:64:PHE:HE1    | 1:A1:86:LEU:CG    | 2.12                     | 0.59              |
| 2:B1:203:ARG:CZ    | 2:B1:230:LEU:HD23 | 2.32                     | 0.59              |
| 1:M1:239:SER:HB2   | 7:S1:18:LEU:HD23  | 1.84                     | 0.59              |
| 1:M1:341:GLN:OE1   | 1:M1:344:ARG:HD3  | 2.03                     | 0.59              |
| 2:N1:76:THR:HG21   | 2:N1:133:ARG:NH2  | 2.18                     | 0.59              |
| 2:N1:206:LEU:HD13  | 2:N1:224:LEU:HD11 | 1.84                     | 0.59              |
| 4:P1:139:THR:HB    | 8:T1:44:VAL:HB    | 1.83                     | 0.59              |
| 5:Q1:104:LYS:HG2   | 5:Q1:104:LYS:O    | 2.01                     | 0.59              |
| 8:T1:58:LEU:HD11   | 8:T1:62:LEU:CD1   | 2.32                     | 0.59              |
| 9:U1:58:GLN:HA     | 9:U1:78:TYR:CD2   | 2.37                     | 0.59              |
| 14:42:60:SER:OG    | 14:42:63:THR:O    | 2.19                     | 0.59              |
| 15:52:49:LEU:HD21  | 16:72:49:GLY:H    | 1.68                     | 0.59              |
| 1:A1:233:PRO:HG2   | 5:E1:23:LYS:HD2   | 1.84                     | 0.59              |
| 3:C1:160:LEU:HD12  | 3:C1:160:LEU:O    | 2.03                     | 0.59              |
| 3:C1:218:ILE:HG21  | 3:C1:223:TYR:CD2  | 2.38                     | 0.59              |
| 4:D1:26:ILE:HG22   | 4:D1:54:VAL:HG13  | 1.84                     | 0.59              |
| 1:M1:233:PRO:HG2   | 5:Q1:23:LYS:CD    | 2.32                     | 0.59              |
| 1:M1:351:GLU:HA    | 1:M1:404:ALA:HB2  | 1.85                     | 0.59              |
| 2:N1:203:ARG:CZ    | 2:N1:230:LEU:HD23 | 2.33                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Q1:40:THR:HG22  | 10:V1:20:PHE:HZ    | 1.67                     | 0.59              |
| 5:Q1:76:ILE:HA    | 5:Q1:193:VAL:O     | 2.03                     | 0.59              |
| 6:R1:58:ARG:HG2   | 6:R1:58:ARG:HH11   | 1.68                     | 0.59              |
| 19:A2:272:ARG:CZ  | 25:G2:87:MET:HE3   | 2.33                     | 0.59              |
| 23:E2:188:GLU:O   | 23:E2:192:ASN:ND2  | 2.36                     | 0.59              |
| 32:O2:33:ARG:NH1  | 40:M2:44:SER:O     | 2.34                     | 0.59              |
| 54:g2:77:CYS:SG   | 54:g2:78:GLN:N     | 2.71                     | 0.59              |
| 2:B1:132:PHE:HB3  | 2:B1:137:VAL:HG21  | 1.85                     | 0.59              |
| 3:C1:25:SER:O     | 3:C1:26:ASN:C      | 2.45                     | 0.59              |
| 3:C1:28:SER:HB3   | 3:C1:30:TRP:HD1    | 1.67                     | 0.59              |
| 3:C1:115:ILE:CD1  | 3:C1:115:ILE:N     | 2.66                     | 0.59              |
| 2:N1:264:ILE:HD12 | 2:N1:315:SER:O     | 2.03                     | 0.59              |
| 3:O1:1:MET:SD     | 3:O1:4:ILE:HB      | 2.43                     | 0.59              |
| 3:O1:221:HIS:HB3  | 3:O1:222:PRO:CD    | 2.29                     | 0.59              |
| 52:12:228:TYR:O   | 52:12:231:ILE:HG22 | 2.03                     | 0.59              |
| 1:A1:62:LEU:O     | 1:A1:63:ALA:C      | 2.46                     | 0.59              |
| 1:A1:436:ARG:HE   | 3:C1:222:PRO:HD3   | 1.68                     | 0.59              |
| 3:C1:8:HIS:CB     | 3:C1:9:PRO:CD      | 2.81                     | 0.59              |
| 3:C1:309:THR:HG21 | 3:C1:367:PRO:O     | 2.03                     | 0.59              |
| 6:F1:42:ASP:O     | 6:F1:43:VAL:C      | 2.43                     | 0.59              |
| 1:M1:46:ARG:NH2   | 1:M1:316:ASP:OD2   | 2.34                     | 0.59              |
| 1:M1:272:VAL:HG21 | 1:M1:402:VAL:HG21  | 1.85                     | 0.59              |
| 2:N1:69:LEU:HD21  | 2:N1:199:PHE:CZ    | 2.37                     | 0.59              |
| 19:A2:469:ALA:HB3 | 19:A2:472:PRO:HG3  | 1.85                     | 0.59              |
| 25:G2:131:LYS:HE3 | 25:G2:147:VAL:HG11 | 1.85                     | 0.59              |
| 54:g2:91:GLN:NE2  | 54:g2:95:ASP:OD2   | 2.36                     | 0.59              |
| 4:D1:168:VAL:O    | 4:D1:169:LEU:HD23  | 2.01                     | 0.59              |
| 7:G1:44:CYS:SG    | 7:G1:48:VAL:CG2    | 2.91                     | 0.59              |
| 1:M1:308:GLN:HG3  | 1:M1:308:GLN:O     | 2.02                     | 0.59              |
| 1:M1:397:SER:O    | 1:M1:400:ALA:HB3   | 2.03                     | 0.59              |
| 2:N1:100:SER:HB3  | 2:N1:105:MET:CG    | 2.32                     | 0.59              |
| 2:N1:384:SER:CB   | 9:U1:62:ARG:HG2    | 2.32                     | 0.59              |
| 3:O1:153:ILE:HD12 | 3:O1:153:ILE:N     | 2.18                     | 0.59              |
| 5:Q1:69:LEU:HG    | 5:Q1:69:LEU:O      | 2.02                     | 0.59              |
| 14:42:52:PHE:O    | 45:b2:135:ARG:NH1  | 2.35                     | 0.59              |
| 1:A1:426:GLY:HA2  | 1:A1:428:ILE:CG1   | 2.32                     | 0.58              |
| 2:B1:247:GLN:HG3  | 2:B1:248:ASN:N     | 2.18                     | 0.58              |
| 1:M1:236:PHE:HD2  | 1:M1:258:GLU:CG    | 2.15                     | 0.58              |
| 2:N1:183:ILE:HG22 | 2:N1:184:GLY:N     | 2.16                     | 0.58              |
| 5:Q1:77:LYS:HG3   | 5:Q1:89:PHE:HE2    | 1.68                     | 0.58              |
| 1:A1:408:ARG:CZ   | 11:K1:15:ARG:NE    | 2.63                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:32:GLN:HG2    | 1:M1:33:PRO:HD2    | 1.84                     | 0.58              |
| 5:Q1:121:GLN:HG3   | 5:Q1:179:ASN:HD22  | 1.67                     | 0.58              |
| 10:V1:51:LEU:H     | 10:V1:54:HIS:HD2   | 1.49                     | 0.58              |
| 14:42:115:LEU:HB2  | 14:42:174:LEU:HD13 | 1.85                     | 0.58              |
| 19:A2:129:PRO:HD2  | 27:I2:114:TYR:CZ   | 2.37                     | 0.58              |
| 1:A1:48:GLU:OE1    | 1:A1:53:ASN:O      | 2.20                     | 0.58              |
| 1:A1:426:GLY:H     | 1:A1:428:ILE:HG13  | 1.63                     | 0.58              |
| 3:C1:4:ILE:HG22    | 3:C1:4:ILE:O       | 2.02                     | 0.58              |
| 3:C1:239:LEU:HD12  | 3:C1:239:LEU:O     | 2.02                     | 0.58              |
| 4:P1:120:ARG:HH11  | 4:P1:120:ARG:CG    | 2.16                     | 0.58              |
| 10:V1:18:SER:HB3   | 11:W1:23:LEU:HD12  | 1.84                     | 0.58              |
| 19:A2:161:GLU:N    | 27:I2:102:ASN:ND2  | 2.37                     | 0.58              |
| 20:B2:92:HIS:O     | 20:B2:94:VAL:N     | 2.35                     | 0.58              |
| 20:B2:305:THR:HG23 | 20:B2:306:GLN:HG2  | 1.85                     | 0.58              |
| 27:I2:107:THR:HB   | 27:I2:121:GLN:O    | 2.03                     | 0.58              |
| 39:V2:50:MET:SD    | 39:V2:54:ASN:ND2   | 2.75                     | 0.58              |
| 45:b2:119:ARG:NH1  | 54:g2:62:TYR:O     | 2.36                     | 0.58              |
| 48:f2:11:THR:H     | 48:f2:14:GLN:HE21  | 1.51                     | 0.58              |
| 1:A1:408:ARG:NH2   | 11:K1:15:ARG:CZ    | 2.64                     | 0.58              |
| 2:B1:169:ARG:HG2   | 2:N1:435:PHE:CE1   | 2.39                     | 0.58              |
| 3:C1:332:LEU:HD21  | 3:C1:358:TYR:CE1   | 2.38                     | 0.58              |
| 6:F1:75:LEU:C      | 6:F1:80:TRP:HE1    | 2.12                     | 0.58              |
| 2:N1:146:ILE:O     | 2:N1:150:VAL:HG13  | 2.03                     | 0.58              |
| 1:A1:120:CYS:O     | 1:A1:122:LEU:HG    | 2.04                     | 0.58              |
| 1:A1:156:THR:OG1   | 1:A1:241:ILE:HB    | 2.03                     | 0.58              |
| 1:A1:268:VAL:O     | 1:A1:272:VAL:HG23  | 2.03                     | 0.58              |
| 3:C1:137:GLN:OE1   | 3:C1:259:ALA:HA    | 2.02                     | 0.58              |
| 4:D1:40:CYS:HB3    | 4:D1:95:TYR:OH     | 2.02                     | 0.58              |
| 4:D1:43:MET:HG2    | 4:D1:46:VAL:CG2    | 2.33                     | 0.58              |
| 4:D1:79:GLU:OE1    | 4:D1:82:MET:HG3    | 2.03                     | 0.58              |
| 3:O1:240:MET:HA    | 3:O1:243:VAL:HG12  | 1.86                     | 0.58              |
| 19:A2:161:GLU:HB3  | 27:I2:102:ASN:CG   | 2.28                     | 0.58              |
| 19:A2:313:LEU:HA   | 38:U2:142:THR:HA   | 1.85                     | 0.58              |
| 21:C2:109:GLN:HE21 | 31:N2:83:GLN:HE22  | 1.50                     | 0.58              |
| 22:D2:64:GLU:HG2   | 22:D2:66:VAL:H     | 1.67                     | 0.58              |
| 1:A1:55:ALA:O      | 1:A1:58:PHE:N      | 2.35                     | 0.58              |
| 2:B1:213:HIS:N     | 2:B1:214:PRO:CD    | 2.66                     | 0.58              |
| 3:C1:51:LEU:HD21   | 3:C1:79:ILE:CG2    | 2.33                     | 0.58              |
| 4:D1:224:ARG:O     | 4:D1:225:HIS:C     | 2.47                     | 0.58              |
| 3:O1:68:HIS:NE2    | 5:Q1:67:ASP:HB2    | 2.18                     | 0.58              |
| 3:O1:320:LEU:HB2   | 3:O1:373:GLU:OE2   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:P1:113:LEU:O    | 4:P1:114:SER:C     | 2.46                     | 0.58              |
| 7:S1:68:LYS:O     | 7:S1:72:LYS:N      | 2.31                     | 0.58              |
| 8:T1:73:LEU:O     | 8:T1:73:LEU:HG     | 2.02                     | 0.58              |
| 10:V1:45:HIS:O    | 10:V1:48:GLU:HG2   | 2.02                     | 0.58              |
| 12:22:21:MET:HE1  | 78:j2:201:PC1:H3B1 | 1.85                     | 0.58              |
| 33:P2:40:LYS:O    | 39:V2:7:LYS:N      | 2.37                     | 0.58              |
| 4:D1:100:ALA:O    | 4:D1:103:ALA:N     | 2.37                     | 0.58              |
| 5:E1:15:ARG:CB    | 5:E1:16:PRO:CD     | 2.79                     | 0.58              |
| 3:O1:15:ASN:O     | 3:O1:18:PHE:HD2    | 1.87                     | 0.58              |
| 3:O1:110:LEU:HG   | 3:O1:114:ASN:HD21  | 1.67                     | 0.58              |
| 5:Q1:153:PHE:CE1  | 5:Q1:172:ARG:HB2   | 2.39                     | 0.58              |
| 5:Q1:188:THR:CG2  | 5:Q1:194:ILE:HG13  | 2.34                     | 0.58              |
| 6:R1:28:LYS:CB    | 6:R1:74:ILE:HD11   | 2.34                     | 0.58              |
| 10:V1:57:HIS:O    | 10:V1:58:LYS:C     | 2.46                     | 0.58              |
| 1:A1:36:THR:OG1   | 1:A1:372:THR:HG22  | 2.03                     | 0.58              |
| 3:C1:67:THR:O     | 3:C1:71:ARG:HG3    | 2.04                     | 0.58              |
| 5:E1:34:GLY:HA2   | 10:J1:10:TYR:HD2   | 1.67                     | 0.58              |
| 7:G1:73:ASN:H     | 7:G1:74:PRO:HD2    | 1.67                     | 0.58              |
| 1:M1:91:THR:CG2   | 1:M1:93:GLU:H      | 2.11                     | 0.58              |
| 3:O1:377:LEU:O    | 3:O1:378:LYS:HB3   | 2.03                     | 0.58              |
| 19:A2:311:LYS:HB2 | 38:U2:142:THR:O    | 2.04                     | 0.58              |
| 2:B1:49:LEU:HD21  | 2:B1:204:MET:SD    | 2.44                     | 0.58              |
| 2:B1:238:LYS:HE3  | 2:B1:239:TYR:O     | 2.04                     | 0.58              |
| 3:C1:51:LEU:CD2   | 3:C1:79:ILE:HG22   | 2.34                     | 0.58              |
| 4:D1:138:PRO:CB   | 8:H1:55:THR:N      | 2.66                     | 0.58              |
| 7:G1:2:ARG:HB2    | 7:G1:6:HIS:CD2     | 2.38                     | 0.58              |
| 8:H1:21:ARG:HB3   | 8:H1:65:ARG:NH2    | 2.17                     | 0.58              |
| 1:M1:233:PRO:HG2  | 5:Q1:23:LYS:NZ     | 2.19                     | 0.58              |
| 2:N1:299:VAL:HG13 | 2:N1:303:VAL:HG21  | 1.86                     | 0.58              |
| 3:O1:163:TRP:O    | 3:O1:177:ARG:NH1   | 2.34                     | 0.58              |
| 3:O1:310:SER:HB3  | 3:O1:318:ARG:NH1   | 2.18                     | 0.58              |
| 4:P1:26:ILE:O     | 4:P1:27:ARG:C      | 2.47                     | 0.58              |
| 4:P1:178:THR:CB   | 4:P1:181:GLN:HG3   | 2.28                     | 0.58              |
| 5:Q1:185:TYR:HA   | 5:Q1:194:ILE:O     | 2.04                     | 0.58              |
| 8:T1:73:LEU:HD21  | 8:T1:74:PHE:HD1    | 1.68                     | 0.58              |
| 26:H2:21:GLN:HB3  | 26:H2:37:GLU:HG3   | 1.85                     | 0.58              |
| 51:j2:108:THR:OG1 | 54:g2:75:THR:O     | 2.21                     | 0.58              |
| 1:A1:24:ARG:CB    | 1:A1:196:VAL:HG22  | 2.25                     | 0.58              |
| 1:A1:311:ASN:OD1  | 1:A1:320:LEU:CD2   | 2.52                     | 0.58              |
| 1:A1:426:GLY:CA   | 1:A1:428:ILE:N     | 2.66                     | 0.58              |
| 2:B1:68:LEU:HD11  | 2:B1:140:LEU:HD23  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B1:72:ALA:O     | 2:B1:75:LEU:HG     | 2.04                     | 0.58              |
| 3:C1:377:LEU:HB3  | 6:F1:33:ARG:HD2    | 1.85                     | 0.58              |
| 2:N1:275:LEU:HD22 | 2:N1:414:ALA:HB2   | 1.85                     | 0.58              |
| 2:N1:280:GLY:HA2  | 2:N1:311:ALA:HB3   | 1.85                     | 0.58              |
| 19:A2:226:CYS:SG  | 75:A2:802:SF4:S3   | 3.02                     | 0.58              |
| 25:G2:154:LYS:HB2 | 25:G2:156:LYS:HE2  | 1.85                     | 0.58              |
| 3:C1:327:ALA:O    | 3:C1:331:ASP:N     | 2.32                     | 0.57              |
| 4:D1:3:LEU:HD22   | 7:G1:70:LYS:NZ     | 2.19                     | 0.57              |
| 4:D1:50:HIS:O     | 4:D1:54:VAL:N      | 2.28                     | 0.57              |
| 9:I1:58:GLN:HG2   | 9:I1:78:TYR:CD2    | 2.38                     | 0.57              |
| 10:J1:38:GLY:O    | 10:J1:42:ILE:HG13  | 2.04                     | 0.57              |
| 1:M1:342:TRP:O    | 1:M1:345:LEU:HB2   | 2.04                     | 0.57              |
| 2:N1:97:SER:OG    | 9:U1:70:LEU:HB2    | 2.04                     | 0.57              |
| 5:Q1:114:VAL:O    | 5:Q1:117:LEU:HB2   | 2.04                     | 0.57              |
| 6:R1:51:PRO:HG2   | 6:R1:54:LEU:HD23   | 1.84                     | 0.57              |
| 34:Q2:168:PHE:H   | 34:Q2:170:TRP:HD1  | 1.52                     | 0.57              |
| 3:C1:316:MET:HE2  | 3:C1:317:PHE:CE1   | 2.40                     | 0.57              |
| 4:D1:178:THR:CB   | 4:D1:181:GLN:HG3   | 2.32                     | 0.57              |
| 1:M1:64:PHE:HE1   | 1:M1:86:LEU:HG     | 1.61                     | 0.57              |
| 2:N1:109:VAL:O    | 2:N1:109:VAL:HG13  | 2.04                     | 0.57              |
| 3:O1:67:THR:O     | 3:O1:71:ARG:HG3    | 2.04                     | 0.57              |
| 3:O1:240:MET:O    | 3:O1:244:LEU:HB2   | 2.04                     | 0.57              |
| 7:S1:50:PRO:CB    | 7:S1:51:PRO:CD     | 2.70                     | 0.57              |
| 8:T1:25:GLU:HA    | 8:T1:30:CYS:SG     | 2.44                     | 0.57              |
| 19:A2:140:GLN:HB2 | 75:A2:801:SF4:S4   | 2.44                     | 0.57              |
| 56:A3:404:THR:O   | 56:A3:480:ARG:NH1  | 2.37                     | 0.57              |
| 57:B3:193:TYR:HE1 | 59:D3:126:MET:HE1  | 1.68                     | 0.57              |
| 2:B1:99:THR:O     | 2:B1:106:ALA:N     | 2.37                     | 0.57              |
| 10:J1:32:GLU:CG   | 10:J1:33:ARG:N     | 2.67                     | 0.57              |
| 1:M1:317:THR:HG22 | 1:M1:318:GLY:N     | 2.19                     | 0.57              |
| 4:P1:10:TYR:O     | 4:P1:12:TRP:CD1    | 2.58                     | 0.57              |
| 6:R1:47:ILE:O     | 6:R1:50:LEU:HG     | 2.04                     | 0.57              |
| 19:A2:302:LEU:CB  | 38:U2:137:TRP:HB3  | 2.34                     | 0.57              |
| 19:A2:456:ALA:HA  | 19:A2:496:ILE:HD13 | 1.86                     | 0.57              |
| 2:B1:248:ASN:HB2  | 2:B1:428:GLY:CA    | 2.33                     | 0.57              |
| 3:C1:221:HIS:CB   | 3:C1:222:PRO:HD3   | 2.22                     | 0.57              |
| 4:D1:138:PRO:HG2  | 8:H1:55:THR:OG1    | 2.04                     | 0.57              |
| 5:E1:33:LYS:HA    | 7:G1:21:PHE:CE2    | 2.38                     | 0.57              |
| 8:H1:35:GLU:O     | 8:H1:39:LEU:HG     | 2.04                     | 0.57              |
| 8:H1:65:ARG:CG    | 8:H1:66:ASP:N      | 2.66                     | 0.57              |
| 1:M1:45:SER:HB3   | 1:M1:167:VAL:HG22  | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:268:VAL:O     | 1:M1:272:VAL:HG23  | 2.04                     | 0.57              |
| 1:M1:270:LEU:O     | 1:M1:273:ALA:HB3   | 2.04                     | 0.57              |
| 1:M1:350:THR:HB    | 1:M1:353:GLU:HG3   | 1.85                     | 0.57              |
| 2:N1:141:GLN:HB2   | 2:N1:142:PRO:HD3   | 1.86                     | 0.57              |
| 2:N1:264:ILE:HG21  | 2:N1:317:SER:HA    | 1.85                     | 0.57              |
| 3:O1:309:THR:HG23  | 3:O1:370:GLY:HA3   | 1.87                     | 0.57              |
| 4:P1:23:HIS:CD2    | 10:V1:51:LEU:HA    | 2.38                     | 0.57              |
| 13:32:64:LEU:HD13  | 16:72:165:VAL:HG22 | 1.85                     | 0.57              |
| 18:92:111:ARG:NH1  | 19:A2:193:ASP:CB   | 2.68                     | 0.57              |
| 19:A2:127:ASP:OD2  | 19:A2:175:ARG:NH1  | 2.36                     | 0.57              |
| 36:S2:193:VAL:HG22 | 36:S2:244:LEU:HB3  | 1.85                     | 0.57              |
| 1:A1:106:LEU:HB3   | 1:A1:107:PRO:HD3   | 1.85                     | 0.57              |
| 3:C1:171:ASP:O     | 3:C1:172:LYS:C     | 2.47                     | 0.57              |
| 1:M1:270:LEU:O     | 1:M1:271:GLN:C     | 2.47                     | 0.57              |
| 1:M1:408:ARG:CZ    | 11:W1:15:ARG:NE    | 2.67                     | 0.57              |
| 3:O1:211:ILE:HG21  | 6:R1:62:ILE:HD13   | 1.86                     | 0.57              |
| 3:O1:310:SER:HB3   | 3:O1:318:ARG:HH11  | 1.70                     | 0.57              |
| 10:V1:34:ALA:O     | 10:V1:35:PHE:C     | 2.46                     | 0.57              |
| 17:82:315:LEU:H    | 17:82:358:ASP:HA   | 1.69                     | 0.57              |
| 19:A2:161:GLU:CA   | 27:I2:102:ASN:HD22 | 2.16                     | 0.57              |
| 20:B2:338:ARG:NH1  | 39:V2:22:LYS:O     | 2.37                     | 0.57              |
| 1:A1:386:TYR:N     | 1:A1:386:TYR:CD1   | 2.72                     | 0.57              |
| 1:A1:417:ASP:OD1   | 5:E1:33:LYS:HD2    | 2.04                     | 0.57              |
| 2:B1:52:LYS:HB2    | 2:B1:203:ARG:CB    | 2.25                     | 0.57              |
| 2:B1:203:ARG:NE    | 2:B1:230:LEU:HD23  | 2.20                     | 0.57              |
| 3:C1:26:ASN:ND2    | 3:C1:26:ASN:C      | 2.63                     | 0.57              |
| 3:C1:372:ILE:O     | 3:C1:373:GLU:C     | 2.46                     | 0.57              |
| 5:E1:29:SER:CB     | 5:E1:32:ARG:HD3    | 2.35                     | 0.57              |
| 6:F1:39:GLU:HB3    | 6:F1:44:LYS:HE2    | 1.87                     | 0.57              |
| 8:H1:58:LEU:HD11   | 8:H1:62:LEU:CD1    | 2.34                     | 0.57              |
| 2:N1:328:SER:HB3   | 2:N1:336:VAL:HG21  | 1.86                     | 0.57              |
| 4:P1:138:PRO:CB    | 8:T1:55:THR:N      | 2.67                     | 0.57              |
| 12:22:176:ARG:O    | 12:22:180:ALA:N    | 2.37                     | 0.57              |
| 16:72:57:PHE:O     | 16:72:62:GLY:N     | 2.37                     | 0.57              |
| 18:92:95:ILE:HD11  | 19:A2:210:ILE:HG23 | 1.79                     | 0.57              |
| 19:A2:667:GLN:NE2  | 29:K2:38:GLU:CD    | 2.62                     | 0.57              |
| 21:C2:230:GLN:HE21 | 21:C2:233:ARG:HH12 | 1.53                     | 0.57              |
| 37:T2:103:ALA:O    | 37:T2:106:ARG:NH1  | 2.37                     | 0.57              |
| 52:12:41:GLY:HA3   | 52:12:44:GLY:H     | 1.69                     | 0.57              |
| 53:62:267:THR:O    | 53:62:274:GLN:NE2  | 2.38                     | 0.57              |
| 57:B3:193:TYR:CE1  | 59:D3:126:MET:HE1  | 2.39                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 66:K3:43:SER:OG    | 66:K3:45:VAL:HG12 | 2.04                     | 0.57              |
| 2:B1:134:ARG:HH12  | 6:R1:51:PRO:HD3   | 1.69                     | 0.57              |
| 3:C1:213:SER:O     | 3:C1:215:VAL:N    | 2.36                     | 0.57              |
| 1:M1:64:PHE:CE1    | 1:M1:86:LEU:CG    | 2.81                     | 0.57              |
| 1:M1:354:VAL:HG13  | 1:M1:407:VAL:HG21 | 1.86                     | 0.57              |
| 2:N1:187:THR:O     | 2:N1:190:GLU:HB2  | 2.05                     | 0.57              |
| 2:N1:304:HIS:CG    | 2:N1:305:GLN:H    | 2.22                     | 0.57              |
| 15:52:96:LEU:HD13  | 53:62:581:LYS:HB3 | 1.86                     | 0.57              |
| 23:E2:66:LEU:HD12  | 23:E2:70:LEU:HD12 | 1.87                     | 0.57              |
| 26:H2:49:SER:HB3   | 45:b2:171:TYR:HB2 | 1.86                     | 0.57              |
| 53:62:247:LEU:HD12 | 53:62:252:MET:HG3 | 1.87                     | 0.57              |
| 55:e2:75:TYR:N     | 55:e2:75:TYR:CD2  | 2.72                     | 0.57              |
| 67:L3:41:ARG:HG3   | 68:M3:40:TYR:CE2  | 2.40                     | 0.57              |
| 1:A1:4:TYR:CE2     | 1:A1:396:GLU:HG3  | 2.38                     | 0.57              |
| 1:A1:143:THR:HG21  | 9:I1:48:SER:N     | 2.14                     | 0.57              |
| 1:A1:248:LEU:N     | 1:A1:248:LEU:HD23 | 2.19                     | 0.57              |
| 1:A1:394:GLU:O     | 1:A1:397:SER:N    | 2.38                     | 0.57              |
| 2:B1:277:HIS:CD2   | 2:B1:364:LEU:HD13 | 2.40                     | 0.57              |
| 1:M1:240:GLN:HG3   | 1:M1:422:VAL:O    | 2.05                     | 0.57              |
| 2:N1:79:GLY:CA     | 2:N1:125:ASN:HD21 | 2.17                     | 0.57              |
| 2:N1:148:LYS:HD2   | 2:N1:178:CYS:O    | 2.04                     | 0.57              |
| 3:O1:218:ILE:HG23  | 3:O1:219:PRO:HD2  | 1.86                     | 0.57              |
| 5:Q1:87:MET:HG2    | 5:Q1:89:PHE:CE1   | 2.40                     | 0.57              |
| 17:82:422:HIS:ND1  | 19:A2:79:LEU:CD1  | 2.67                     | 0.57              |
| 19:A2:272:ARG:CZ   | 25:G2:87:MET:CE   | 2.82                     | 0.57              |
| 3:C1:71:ARG:NH2    | 4:D1:193:ALA:O    | 2.38                     | 0.57              |
| 1:M1:270:LEU:O     | 1:M1:273:ALA:N    | 2.38                     | 0.57              |
| 3:O1:149:LEU:HD21  | 3:O1:281:LEU:HD22 | 1.86                     | 0.57              |
| 4:P1:240:PRO:CD    | 4:P1:241:LYS:H    | 2.16                     | 0.57              |
| 19:A2:422:TRP:CD2  | 25:G2:169:ARG:HD3 | 2.40                     | 0.57              |
| 20:B2:97:LEU:CB    | 20:B2:111:PRO:HA  | 2.35                     | 0.57              |
| 20:B2:263:THR:O    | 20:B2:269:ARG:NH2 | 2.37                     | 0.57              |
| 20:B2:357:LYS:HD3  | 20:B2:364:SER:HB2 | 1.87                     | 0.57              |
| 22:D2:113:PHE:N    | 22:D2:113:PHE:CD1 | 2.73                     | 0.57              |
| 3:C1:28:SER:HB3    | 3:C1:30:TRP:CD1   | 2.40                     | 0.57              |
| 2:N1:59:ASN:CG     | 2:N1:60:SER:H     | 2.11                     | 0.57              |
| 2:N1:79:GLY:HA3    | 2:N1:125:ASN:HD21 | 1.70                     | 0.57              |
| 2:N1:206:LEU:HD13  | 2:N1:224:LEU:CD1  | 2.34                     | 0.57              |
| 2:N1:352:LEU:HD12  | 2:N1:353:SER:N    | 2.20                     | 0.57              |
| 3:O1:28:SER:HB3    | 3:O1:30:TRP:CD1   | 2.38                     | 0.57              |
| 3:O1:270:PRO:HB2   | 3:O1:274:PHE:HB2  | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:P1:161:ALA:HB1   | 4:P1:162:PRO:HD2   | 1.86                     | 0.57              |
| 5:Q1:20:ASP:O      | 5:Q1:21:SER:C      | 2.46                     | 0.57              |
| 5:Q1:121:GLN:HG3   | 5:Q1:179:ASN:ND2   | 2.20                     | 0.57              |
| 6:R1:28:LYS:HB3    | 6:R1:74:ILE:HD11   | 1.86                     | 0.57              |
| 56:A3:184:PHE:H    | 56:A3:256:HIS:HE1  | 1.52                     | 0.57              |
| 57:B3:132:GLU:HB3  | 57:B3:137:GLU:HG3  | 1.87                     | 0.57              |
| 57:B3:145:PRO:HG3  | 57:B3:148:MET:HE2  | 1.87                     | 0.57              |
| 57:B3:189:PRO:HD2  | 64:I3:54:TYR:OH    | 2.05                     | 0.57              |
| 3:C1:215:VAL:O     | 6:F1:63:LYS:NZ     | 2.37                     | 0.56              |
| 8:H1:34:ARG:O      | 8:H1:38:GLU:HG2    | 2.05                     | 0.56              |
| 1:M1:18:GLN:HG2    | 1:M1:19:LEU:O      | 2.04                     | 0.56              |
| 1:M1:32:GLN:HG2    | 1:M1:33:PRO:CD     | 2.35                     | 0.56              |
| 1:M1:134:ILE:HA    | 1:M1:137:GLU:HG3   | 1.87                     | 0.56              |
| 2:N1:141:GLN:HE22  | 2:N1:186:VAL:HB    | 1.70                     | 0.56              |
| 2:N1:262:ALA:HB2   | 2:N1:272:PHE:HE2   | 1.69                     | 0.56              |
| 2:N1:303:VAL:CG1   | 2:N1:304:HIS:N     | 2.67                     | 0.56              |
| 2:N1:304:HIS:CG    | 2:N1:305:GLN:N     | 2.72                     | 0.56              |
| 5:Q1:12:ASP:O      | 7:S1:24:ARG:NH2    | 2.32                     | 0.56              |
| 16:72:57:PHE:HA    | 16:72:61:LEU:HB3   | 1.87                     | 0.56              |
| 19:A2:121:LEU:HD21 | 19:A2:139:LEU:HD22 | 1.87                     | 0.56              |
| 19:A2:306:MET:CE   | 38:U2:139:PRO:HG3  | 2.32                     | 0.56              |
| 1:A1:55:ALA:O      | 1:A1:56:GLY:C      | 2.48                     | 0.56              |
| 1:A1:86:LEU:HD13   | 1:A1:99:ILE:CD1    | 2.35                     | 0.56              |
| 1:A1:425:PHE:O     | 1:A1:426:GLY:O     | 2.23                     | 0.56              |
| 1:A1:436:ARG:HE    | 3:C1:222:PRO:CD    | 2.18                     | 0.56              |
| 2:B1:160:ILE:HD11  | 2:B1:325:TYR:CE2   | 2.40                     | 0.56              |
| 1:M1:161:THR:CB    | 1:M1:162:PRO:HD2   | 2.34                     | 0.56              |
| 3:O1:107:TYR:OH    | 3:O1:308:HIS:ND1   | 2.09                     | 0.56              |
| 5:Q1:147:ILE:N     | 5:Q1:157:TYR:O     | 2.36                     | 0.56              |
| 73:42:501:CDL:H312 | 49:h2:107:ALA:HA   | 1.86                     | 0.56              |
| 19:A2:381:LEU:HD21 | 19:A2:664:TYR:HB2  | 1.87                     | 0.56              |
| 19:A2:624:ARG:NH1  | 19:A2:634:LEU:O    | 2.37                     | 0.56              |
| 20:B2:198:THR:HG22 | 52:12:32:GLN:HE22  | 1.70                     | 0.56              |
| 53:62:174:TYR:HB3  | 53:62:229:LEU:HD23 | 1.87                     | 0.56              |
| 1:A1:142:ASP:OD1   | 5:E1:2:HIS:ND1     | 2.36                     | 0.56              |
| 2:B1:237:ALA:HB2   | 2:B1:318:ASP:CG    | 2.31                     | 0.56              |
| 3:C1:225:THR:O     | 3:C1:229:ILE:HD12  | 2.05                     | 0.56              |
| 4:D1:115:TYR:HD2   | 4:D1:119:ALA:HB2   | 1.69                     | 0.56              |
| 4:D1:139:THR:HB    | 8:H1:44:VAL:HB     | 1.86                     | 0.56              |
| 4:D1:150:ASN:OD1   | 4:D1:151:PRO:CD    | 2.53                     | 0.56              |
| 4:D1:223:LYS:HZ2   | 4:D1:227:TRP:CD1   | 2.23                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D1:229:VAL:CG1   | 4:D1:233:ARG:HE   | 2.18                     | 0.56              |
| 6:F1:28:LYS:HD2    | 6:F1:74:ILE:HD11  | 1.88                     | 0.56              |
| 6:F1:74:ILE:HD13   | 6:F1:80:TRP:CZ2   | 2.40                     | 0.56              |
| 10:J1:57:HIS:O     | 10:J1:58:LYS:C    | 2.46                     | 0.56              |
| 10:J1:60:GLU:HG3   | 10:J1:60:GLU:O    | 2.06                     | 0.56              |
| 1:M1:417:ASP:OD1   | 5:Q1:33:LYS:HD2   | 2.05                     | 0.56              |
| 2:N1:68:LEU:HD23   | 2:N1:186:VAL:HG11 | 1.87                     | 0.56              |
| 2:N1:217:LYS:O     | 2:N1:221:GLU:HG3  | 2.05                     | 0.56              |
| 3:O1:88:SER:HA     | 3:O1:272:TRP:HZ2  | 1.70                     | 0.56              |
| 3:O1:313:ARG:HB3   | 6:R1:38:HIS:CD2   | 2.40                     | 0.56              |
| 4:P1:7:PRO:HG3     | 4:P1:126:TYR:CA   | 2.36                     | 0.56              |
| 4:P1:117:VAL:HG11  | 4:P1:191:ARG:HH11 | 1.70                     | 0.56              |
| 9:U1:58:GLN:HG2    | 9:U1:78:TYR:CD2   | 2.40                     | 0.56              |
| 17:82:382:CYS:HB3  | 17:82:384:PRO:HD2 | 1.88                     | 0.56              |
| 19:A2:140:GLN:HA   | 20:B2:379:ILE:CG2 | 2.35                     | 0.56              |
| 19:A2:302:LEU:CA   | 38:U2:137:TRP:HB3 | 2.32                     | 0.56              |
| 20:B2:305:THR:OG1  | 21:C2:140:ASN:ND2 | 2.39                     | 0.56              |
| 46:c2:14:GLN:NE2   | 48:f2:155:PRO:O   | 2.37                     | 0.56              |
| 1:A1:309:THR:HA    | 1:A1:322:ALA:HA   | 1.86                     | 0.56              |
| 1:A1:335:MET:HE2   | 1:A1:339:GLN:HG3  | 1.88                     | 0.56              |
| 1:A1:354:VAL:HG21  | 1:A1:404:ALA:HA   | 1.87                     | 0.56              |
| 2:B1:239:TYR:OH    | 2:B1:421:ARG:O    | 2.19                     | 0.56              |
| 4:D1:181:GLN:HA    | 8:H1:77:LEU:HD13  | 1.87                     | 0.56              |
| 8:H1:21:ARG:CB     | 8:H1:65:ARG:HH21  | 2.18                     | 0.56              |
| 1:M1:111:GLU:HG2   | 1:M1:213:GLN:HE22 | 1.71                     | 0.56              |
| 1:M1:434:TYR:HA    | 1:M1:437:ILE:HD12 | 1.87                     | 0.56              |
| 3:O1:18:PHE:O      | 3:O1:220:PHE:CD2  | 2.58                     | 0.56              |
| 3:O1:165:TRP:HA    | 3:O1:174:THR:OG1  | 2.04                     | 0.56              |
| 6:R1:98:ILE:O      | 6:R1:99:ARG:C     | 2.47                     | 0.56              |
| 60:E3:78:HIS:ND1   | 64:I3:12:LEU:HD22 | 2.21                     | 0.56              |
| 62:G3:5:LYS:HD2    | 62:G3:6:GLY:N     | 2.21                     | 0.56              |
| 63:H3:71:THR:O     | 63:H3:75:ARG:HD3  | 2.05                     | 0.56              |
| 1:A1:272:VAL:HG13  | 1:A1:358:LYS:HA   | 1.88                     | 0.56              |
| 3:C1:182:HIS:O     | 3:C1:186:PRO:HD2  | 2.06                     | 0.56              |
| 4:D1:74:PRO:O      | 4:D1:79:GLU:N     | 2.36                     | 0.56              |
| 4:D1:113:LEU:O     | 4:D1:114:SER:C    | 2.48                     | 0.56              |
| 1:M1:349:ALA:HB3   | 1:M1:408:ARG:CG   | 2.35                     | 0.56              |
| 3:O1:34:GLY:O      | 3:O1:37:LEU:HB2   | 2.06                     | 0.56              |
| 4:P1:43:MET:HE3    | 4:P1:91:PHE:CD2   | 2.41                     | 0.56              |
| 4:P1:158:ILE:HG12  | 4:P1:159:GLY:N    | 2.19                     | 0.56              |
| 20:B2:116:LEU:HD23 | 20:B2:118:ARG:HE  | 1.70                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B1:47:ILE:CD1    | 2:B1:120:MET:SD   | 2.93                     | 0.56              |
| 2:B1:89:ILE:O      | 2:B1:90:GLU:C     | 2.47                     | 0.56              |
| 2:B1:102:ARG:HH12  | 2:B1:175:SER:HA   | 1.71                     | 0.56              |
| 3:C1:300:ILE:CD1   | 3:C1:362:ILE:HG21 | 2.36                     | 0.56              |
| 3:C1:337:TRP:O     | 3:C1:338:ILE:C    | 2.48                     | 0.56              |
| 6:F1:73:GLN:HA     | 7:G1:39:ARG:HH21  | 1.71                     | 0.56              |
| 10:J1:12:LEU:HD23  | 10:J1:13:LEU:CD2  | 2.36                     | 0.56              |
| 1:M1:33:PRO:O      | 1:M1:103:SER:N    | 2.34                     | 0.56              |
| 1:M1:134:ILE:CG2   | 1:M1:174:VAL:HG21 | 2.35                     | 0.56              |
| 2:N1:294:SER:HB3   | 2:N1:343:GLN:HE21 | 1.70                     | 0.56              |
| 3:O1:296:PHE:O     | 3:O1:300:ILE:HB   | 2.05                     | 0.56              |
| 4:P1:182:VAL:O     | 4:P1:186:VAL:HG23 | 2.05                     | 0.56              |
| 5:Q1:102:THR:OG1   | 5:Q1:105:GLU:HB2  | 2.06                     | 0.56              |
| 13:32:102:LEU:O    | 13:32:106:TRP:N   | 2.38                     | 0.56              |
| 17:82:159:ARG:HG2  | 17:82:161:GLU:H   | 1.71                     | 0.56              |
| 1:A1:278:GLY:O     | 1:A1:309:THR:HG23 | 2.05                     | 0.56              |
| 2:B1:264:ILE:CG2   | 2:B1:317:SER:HA   | 2.36                     | 0.56              |
| 2:B1:273:SER:O     | 2:B1:276:GLN:HB3  | 2.06                     | 0.56              |
| 2:B1:280:GLY:HA2   | 2:B1:311:ALA:HB3  | 1.88                     | 0.56              |
| 4:D1:21:LEU:CD1    | 4:D1:192:TRP:HB2  | 2.36                     | 0.56              |
| 4:D1:79:GLU:O      | 4:D1:80:MET:C     | 2.49                     | 0.56              |
| 1:M1:64:PHE:HA     | 1:M1:75:LEU:CD2   | 2.35                     | 0.56              |
| 1:M1:334:MET:HE3   | 1:M1:334:MET:HA   | 1.86                     | 0.56              |
| 3:O1:300:ILE:O     | 3:O1:300:ILE:HG12 | 2.05                     | 0.56              |
| 3:O1:327:ALA:O     | 3:O1:331:ASP:N    | 2.35                     | 0.56              |
| 7:S1:31:SER:O      | 7:S1:35:PRO:CD    | 2.47                     | 0.56              |
| 13:32:81:THR:H     | 30:L2:46:ASN:HD21 | 1.53                     | 0.56              |
| 14:42:451:PRO:HG2  | 53:62:69:LEU:HD23 | 1.88                     | 0.56              |
| 17:82:411:SER:HB3  | 33:P2:49:LEU:HD13 | 1.86                     | 0.56              |
| 17:82:419:ILE:HD11 | 19:A2:119:PHE:CE2 | 2.41                     | 0.56              |
| 41:X2:37:PHE:HD2   | 45:b2:137:MET:HB3 | 1.69                     | 0.56              |
| 58:C3:203:PHE:O    | 58:C3:207:HIS:HD2 | 1.88                     | 0.56              |
| 3:C1:41:LEU:O      | 3:C1:45:ILE:HG13  | 2.06                     | 0.56              |
| 6:F1:50:LEU:CB     | 6:F1:55:TYR:HB2   | 2.29                     | 0.56              |
| 2:N1:318:ASP:OD1   | 2:N1:318:ASP:N    | 2.39                     | 0.56              |
| 3:O1:185:LEU:HB3   | 3:O1:186:PRO:CD   | 2.35                     | 0.56              |
| 4:P1:21:LEU:HD11   | 4:P1:192:TRP:HB2  | 1.88                     | 0.56              |
| 4:P1:180:SER:HB3   | 8:T1:17:LEU:HB2   | 1.88                     | 0.56              |
| 17:82:159:ARG:NH1  | 18:92:176:CYS:O   | 2.38                     | 0.56              |
| 19:A2:130:ILE:HG12 | 27:I2:114:TYR:CZ  | 2.41                     | 0.56              |
| 19:A2:313:LEU:HD23 | 38:U2:142:THR:CB  | 2.31                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:e2:77:LYS:CG    | 55:e2:78:LEU:N     | 2.68                     | 0.56              |
| 1:A1:106:LEU:HD22  | 1:A1:203:LEU:CD2   | 2.31                     | 0.56              |
| 1:A1:272:VAL:HG21  | 1:A1:402:VAL:HG21  | 1.87                     | 0.56              |
| 3:C1:133:LEU:HD21  | 3:C1:179:PHE:HA    | 1.88                     | 0.56              |
| 3:C1:338:ILE:CD1   | 3:C1:338:ILE:H     | 2.19                     | 0.56              |
| 5:E1:31:ALA:HB1    | 10:J1:6:THR:OG1    | 2.05                     | 0.56              |
| 5:E1:45:VAL:HG13   | 10:J1:28:ALA:N     | 2.21                     | 0.56              |
| 6:F1:91:GLU:HB2    | 6:F1:92:PRO:HD3    | 1.86                     | 0.56              |
| 2:N1:264:ILE:HB    | 2:N1:316:TYR:O     | 2.06                     | 0.56              |
| 3:O1:108:THR:CB    | 3:O1:313:ARG:HH11  | 2.12                     | 0.56              |
| 3:O1:218:ILE:CG2   | 3:O1:223:TYR:HD2   | 2.19                     | 0.56              |
| 5:Q1:142:LEU:HD12  | 5:Q1:161:HIS:HE1   | 1.71                     | 0.56              |
| 19:A2:140:GLN:HA   | 20:B2:379:ILE:HG21 | 1.87                     | 0.56              |
| 1:A1:146:ARG:CZ    | 1:A1:308:GLN:HE22  | 2.19                     | 0.56              |
| 2:B1:24:LEU:H      | 2:B1:24:LEU:CD1    | 2.03                     | 0.56              |
| 2:B1:55:SER:OG     | 2:B1:102:ARG:HG2   | 2.06                     | 0.56              |
| 3:C1:221:HIS:HB3   | 3:C1:222:PRO:CD    | 2.27                     | 0.56              |
| 3:C1:236:ILE:O     | 3:C1:237:LEU:C     | 2.48                     | 0.56              |
| 4:D1:228:SER:HB2   | 7:G1:23:GLN:HE22   | 1.71                     | 0.56              |
| 1:M1:233:PRO:HG2   | 5:Q1:23:LYS:CE     | 2.36                     | 0.56              |
| 2:N1:264:ILE:HG22  | 2:N1:317:SER:HA    | 1.88                     | 0.56              |
| 2:N1:308:ASP:OD2   | 9:U1:55:LEU:HA     | 2.06                     | 0.56              |
| 3:O1:274:PHE:O     | 3:O1:275:LEU:C     | 2.47                     | 0.56              |
| 5:Q1:76:ILE:O      | 5:Q1:77:LYS:HG2    | 2.06                     | 0.56              |
| 5:Q1:140:THR:HG21  | 5:Q1:178:LEU:HB2   | 1.88                     | 0.56              |
| 8:T1:66:ASP:O      | 8:T1:67:HIS:C      | 2.49                     | 0.56              |
| 18:92:56:THR:HG22  | 18:92:58:GLU:H     | 1.70                     | 0.56              |
| 19:A2:313:LEU:HG   | 38:U2:142:THR:HA   | 1.87                     | 0.56              |
| 19:A2:349:GLU:HG2  | 19:A2:646:LEU:HD11 | 1.88                     | 0.56              |
| 19:A2:588:ALA:O    | 19:A2:592:LYS:NZ   | 2.39                     | 0.56              |
| 19:A2:645:ARG:NH1  | 19:A2:648:GLU:OE1  | 2.39                     | 0.56              |
| 19:A2:667:GLN:HB3  | 29:K2:42:VAL:HB    | 1.87                     | 0.56              |
| 1:A1:25:VAL:HG21   | 1:A1:209:LEU:HD12  | 1.87                     | 0.55              |
| 3:C1:115:ILE:N     | 3:C1:115:ILE:HD12  | 2.21                     | 0.55              |
| 3:C1:218:ILE:HG22  | 3:C1:219:PRO:N     | 2.20                     | 0.55              |
| 4:D1:69:GLU:HA     | 4:D1:73:GLY:HA2    | 1.88                     | 0.55              |
| 9:I1:53:GLU:O      | 9:I1:54:SER:C      | 2.47                     | 0.55              |
| 2:N1:435:PHE:HB2   | 2:N1:438:GLU:OE1   | 2.05                     | 0.55              |
| 3:O1:24:PRO:HG2    | 3:O1:205:SER:O     | 2.06                     | 0.55              |
| 14:42:193:VAL:HG22 | 14:42:257:MET:HE1  | 1.87                     | 0.55              |
| 19:A2:111:LYS:HD2  | 33:P2:53:TYR:CE2   | 2.41                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:A2:111:LYS:CD  | 33:P2:53:TYR:CE2   | 2.89                     | 0.55              |
| 19:A2:129:PRO:HB2 | 27:I2:114:TYR:HE1  | 1.72                     | 0.55              |
| 20:B2:295:GLY:HA2 | 20:B2:321:GLY:H    | 1.72                     | 0.55              |
| 35:R2:238:GLN:HB3 | 35:R2:267:GLY:HA3  | 1.87                     | 0.55              |
| 3:C1:72:ASP:HB3   | 5:E1:67:ASP:H      | 1.71                     | 0.55              |
| 4:D1:27:ARG:NH1   | 10:J1:58:LYS:HG3   | 2.18                     | 0.55              |
| 4:D1:35:GLN:HB2   | 4:D1:169:LEU:CD1   | 2.35                     | 0.55              |
| 1:M1:335:MET:CE   | 1:M1:339:GLN:HG3   | 2.35                     | 0.55              |
| 2:N1:62:ASN:O     | 2:N1:62:ASN:ND2    | 2.39                     | 0.55              |
| 2:N1:342:ASN:O    | 2:N1:345:LYS:HB2   | 2.06                     | 0.55              |
| 4:P1:138:PRO:O    | 4:P1:141:VAL:HB    | 2.06                     | 0.55              |
| 4:P1:139:THR:HG21 | 8:T1:41:ASP:O      | 2.06                     | 0.55              |
| 5:Q1:139:CYS:HB2  | 5:Q1:165:TYR:CE2   | 2.39                     | 0.55              |
| 5:Q1:150:ALA:HB3  | 5:Q1:157:TYR:CB    | 2.36                     | 0.55              |
| 14:42:278:ARG:H   | 53:62:546:GLN:HE22 | 1.54                     | 0.55              |
| 20:B2:237:PRO:HD3 | 23:E2:96:ARG:HH22  | 1.70                     | 0.55              |
| 35:R2:84:HIS:HD2  | 35:R2:87:GLU:H     | 1.52                     | 0.55              |
| 37:T2:78:ALA:HA   | 37:T2:89:ASN:HD21  | 1.71                     | 0.55              |
| 1:A1:136:GLN:HE21 | 9:I1:50:LEU:HB3    | 1.70                     | 0.55              |
| 6:F1:101:ARG:HG2  | 6:F1:105:GLU:OE2   | 2.06                     | 0.55              |
| 3:O1:148:ASN:O    | 3:O1:151:SER:OG    | 2.24                     | 0.55              |
| 5:Q1:50:ALA:O     | 5:Q1:51:ALA:C      | 2.49                     | 0.55              |
| 9:U1:62:ARG:H     | 9:U1:63:PRO:HD2    | 1.71                     | 0.55              |
| 9:U1:70:LEU:HD21  | 9:U1:73:PRO:CD     | 2.26                     | 0.55              |
| 31:N2:35:LEU:O    | 31:N2:45:ARG:NH2   | 2.40                     | 0.55              |
| 32:O2:92:GLU:HG3  | 32:O2:97:TRP:HE3   | 1.72                     | 0.55              |
| 47:d2:25:PHE:CZ   | 47:d2:42:THR:O     | 2.57                     | 0.55              |
| 52:12:230:ASN:HA  | 52:12:233:MET:HE2  | 1.88                     | 0.55              |
| 4:D1:50:HIS:O     | 4:D1:51:LEU:C      | 2.48                     | 0.55              |
| 6:F1:51:PRO:CD    | 2:N1:134:ARG:NH1   | 2.68                     | 0.55              |
| 1:M1:245:GLU:O    | 1:M1:247:GLY:N     | 2.39                     | 0.55              |
| 3:O1:109:PHE:O    | 3:O1:110:LEU:C     | 2.49                     | 0.55              |
| 19:A2:303:THR:CG2 | 38:U2:136:GLU:HA   | 2.37                     | 0.55              |
| 58:C3:42:LEU:HD13 | 65:J3:45:TYR:CD2   | 2.41                     | 0.55              |
| 1:A1:33:PRO:O     | 1:A1:103:SER:N     | 2.36                     | 0.55              |
| 3:C1:135:TRP:HH2  | 3:C1:170:VAL:O     | 1.89                     | 0.55              |
| 3:C1:137:GLN:HB2  | 3:C1:257:THR:OG1   | 2.07                     | 0.55              |
| 3:C1:244:LEU:HD11 | 4:D1:204:MET:CE    | 2.37                     | 0.55              |
| 4:D1:69:GLU:O     | 4:D1:73:GLY:HA3    | 2.05                     | 0.55              |
| 4:D1:229:VAL:O    | 4:D1:233:ARG:HG3   | 2.06                     | 0.55              |
| 6:F1:10:SER:OG    | 6:F1:13:LEU:HD11   | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F1:49:ARG:HD3    | 2:N1:135:TRP:CD2   | 2.41                     | 0.55              |
| 8:H1:73:LEU:HD23   | 8:H1:73:LEU:C      | 2.31                     | 0.55              |
| 1:M1:338:LEU:O     | 1:M1:341:GLN:N     | 2.38                     | 0.55              |
| 1:M1:438:ARG:HH11  | 1:M1:438:ARG:HG3   | 1.70                     | 0.55              |
| 2:N1:92:VAL:O      | 2:N1:92:VAL:HG12   | 2.06                     | 0.55              |
| 3:O1:234:LEU:HD21  | 4:P1:216:LEU:HD21  | 1.86                     | 0.55              |
| 4:P1:7:PRO:CB      | 4:P1:125:ASP:HB3   | 2.37                     | 0.55              |
| 4:P1:149:PHE:HZ    | 8:T1:55:THR:HG23   | 1.71                     | 0.55              |
| 6:R1:106:GLU:OE1   | 6:R1:109:LYS:HE2   | 2.06                     | 0.55              |
| 17:82:156:ILE:HD11 | 17:82:197:VAL:HG22 | 1.88                     | 0.55              |
| 35:R2:92:MET:HG3   | 35:R2:95:ARG:HH21  | 1.71                     | 0.55              |
| 1:A1:93:GLU:O      | 1:A1:94:HIS:ND1    | 2.40                     | 0.55              |
| 3:C1:218:ILE:HG22  | 3:C1:223:TYR:HD2   | 1.72                     | 0.55              |
| 3:C1:353:LEU:HD23  | 3:C1:353:LEU:N     | 2.22                     | 0.55              |
| 5:E1:72:SER:O      | 5:E1:73:LYS:HG2    | 2.05                     | 0.55              |
| 1:M1:334:MET:O     | 1:M1:335:MET:C     | 2.48                     | 0.55              |
| 2:N1:213:HIS:N     | 2:N1:214:PRO:CD    | 2.69                     | 0.55              |
| 2:N1:359:ALA:O     | 2:N1:360:ALA:C     | 2.50                     | 0.55              |
| 3:O1:44:GLN:HE22   | 3:O1:86:GLY:HA3    | 1.70                     | 0.55              |
| 3:O1:315:MET:HA    | 3:O1:318:ARG:HG3   | 1.87                     | 0.55              |
| 5:Q1:188:THR:HG21  | 5:Q1:194:ILE:HD11  | 1.87                     | 0.55              |
| 10:V1:47:ASN:HB3   | 10:V1:50:LYS:HD2   | 1.88                     | 0.55              |
| 15:52:61:ILE:HG23  | 16:72:55:MET:HE1   | 1.89                     | 0.55              |
| 19:A2:180:THR:HA   | 19:A2:183:ILE:HD12 | 1.89                     | 0.55              |
| 19:A2:651:PRO:HD2  | 29:K2:56:ARG:HB3   | 1.89                     | 0.55              |
| 56:A3:95:PRO:HB2   | 58:C3:11:VAL:HG13  | 1.87                     | 0.55              |
| 1:A1:30:SER:N      | 1:A1:201:GLY:O     | 2.38                     | 0.55              |
| 2:B1:100:SER:CB    | 2:B1:105:MET:HG3   | 2.37                     | 0.55              |
| 2:B1:261:SER:OG    | 2:B1:262:ALA:N     | 2.39                     | 0.55              |
| 4:D1:164:ILE:HD11  | 70:D1:301:HEC:CBB  | 2.37                     | 0.55              |
| 10:J1:35:PHE:O     | 10:J1:36:ASP:C     | 2.50                     | 0.55              |
| 1:M1:331:ILE:CD1   | 1:M1:427:PRO:O     | 2.55                     | 0.55              |
| 2:N1:168:TYR:HB2   | 2:N1:173:ALA:HB2   | 1.88                     | 0.55              |
| 3:O1:122:THR:HG22  | 3:O1:189:ILE:CD1   | 2.27                     | 0.55              |
| 3:O1:206:ASN:ND2   | 3:O1:207:ASN:H     | 2.04                     | 0.55              |
| 3:O1:210:GLY:CA    | 3:O1:314:SER:HB2   | 2.31                     | 0.55              |
| 7:S1:33:GLY:O      | 7:S1:37:VAL:N      | 2.35                     | 0.55              |
| 18:92:88:ARG:NH1   | 24:F2:82:THR:O     | 2.39                     | 0.55              |
| 19:A2:303:THR:HG21 | 38:U2:136:GLU:CB   | 2.37                     | 0.55              |
| 19:A2:583:ILE:HD13 | 38:U2:137:TRP:HZ3  | 1.71                     | 0.55              |
| 20:B2:92:HIS:HE1   | 20:B2:141:TYR:HE2  | 1.54                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:B2:348:LEU:HA  | 20:B2:351:MET:HE2  | 1.88                     | 0.55              |
| 23:E2:39:LYS:HG3  | 33:P2:111:PRO:HA   | 1.88                     | 0.55              |
| 1:A1:342:TRP:O    | 1:A1:345:LEU:N     | 2.40                     | 0.55              |
| 1:A1:385:THR:CG2  | 1:A1:386:TYR:CD1   | 2.89                     | 0.55              |
| 1:A1:397:SER:O    | 1:A1:400:ALA:HB3   | 2.07                     | 0.55              |
| 2:B1:86:THR:CG2   | 9:I1:71:ASN:HD21   | 2.19                     | 0.55              |
| 2:B1:203:ARG:NH2  | 2:B1:230:LEU:HD23  | 2.22                     | 0.55              |
| 4:D1:178:THR:O    | 4:D1:179:MET:C     | 2.50                     | 0.55              |
| 4:D1:236:ALA:O    | 7:G1:14:ILE:N      | 2.27                     | 0.55              |
| 5:E1:15:ARG:NH2   | 5:E1:32:ARG:HG3    | 2.22                     | 0.55              |
| 1:M1:67:THR:CG2   | 1:M1:70:ARG:H      | 2.03                     | 0.55              |
| 1:M1:266:ASP:O    | 1:M1:270:LEU:HG    | 2.06                     | 0.55              |
| 2:N1:33:LEU:O     | 2:N1:33:LEU:HD23   | 2.07                     | 0.55              |
| 2:N1:155:PRO:HB2  | 2:N1:254:HIS:CE1   | 2.41                     | 0.55              |
| 2:N1:198:HIS:HE1  | 2:N1:233:SER:OG    | 1.89                     | 0.55              |
| 3:O1:147:THR:O    | 3:O1:150:LEU:HB2   | 2.07                     | 0.55              |
| 4:P1:4:GLU:HG3    | 4:P1:6:HIS:CE1     | 2.42                     | 0.55              |
| 5:Q1:118:ARG:HB3  | 5:Q1:171:ILE:CG2   | 2.36                     | 0.55              |
| 5:Q1:136:ILE:O    | 5:Q1:136:ILE:CG2   | 2.55                     | 0.55              |
| 14:42:452:LYS:NZ  | 49:h2:115:GLN:OE1  | 2.40                     | 0.55              |
| 16:72:66:VAL:O    | 16:72:70:TYR:N     | 2.40                     | 0.55              |
| 56:A3:407:ASP:O   | 56:A3:411:LYS:HG3  | 2.07                     | 0.55              |
| 62:G3:5:LYS:HD2   | 62:G3:5:LYS:C      | 2.32                     | 0.55              |
| 1:A1:112:LEU:O    | 1:A1:116:ILE:HD12  | 2.07                     | 0.55              |
| 2:B1:161:GLU:OE1  | 2:B1:175:SER:HB2   | 2.07                     | 0.55              |
| 3:C1:312:GLN:O    | 3:C1:314:SER:N     | 2.40                     | 0.55              |
| 4:D1:74:PRO:HG2   | 4:D1:82:MET:HB3    | 1.89                     | 0.55              |
| 4:D1:211:MET:HA   | 4:D1:211:MET:HE3   | 1.89                     | 0.55              |
| 1:M1:249:PRO:O    | 1:M1:250:LEU:HD23  | 2.07                     | 0.55              |
| 1:M1:256:ALA:HB3  | 1:M1:421:ALA:HB3   | 1.89                     | 0.55              |
| 3:O1:244:LEU:HD11 | 4:P1:204:MET:CE    | 2.36                     | 0.55              |
| 3:O1:371:THR:O    | 3:O1:372:ILE:C     | 2.49                     | 0.55              |
| 4:P1:42:SER:HB3   | 4:P1:94:PRO:HD2    | 1.89                     | 0.55              |
| 19:A2:139:LEU:O   | 20:B2:379:ILE:HD13 | 2.07                     | 0.55              |
| 19:A2:427:LEU:H   | 25:G2:169:ARG:HH22 | 1.55                     | 0.55              |
| 3:C1:15:ASN:O     | 3:C1:18:PHE:HD1    | 1.90                     | 0.55              |
| 3:C1:71:ARG:HE    | 4:D1:196:PRO:HG3   | 1.72                     | 0.55              |
| 3:C1:251:GLY:O    | 3:C1:252:ASP:C     | 2.50                     | 0.55              |
| 3:C1:310:SER:CB   | 3:C1:318:ARG:NH1   | 2.58                     | 0.55              |
| 4:D1:219:VAL:HA   | 4:D1:222:MET:HG3   | 1.88                     | 0.55              |
| 5:E1:12:ASP:O     | 7:G1:24:ARG:NH2    | 2.35                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:M1:112:LEU:O     | 1:M1:116:ILE:HG13 | 2.07                     | 0.55              |
| 2:N1:155:PRO:O     | 2:N1:156:GLN:C    | 2.49                     | 0.55              |
| 3:O1:119:LEU:HD13  | 3:O1:192:ILE:CG2  | 2.37                     | 0.55              |
| 3:O1:132:VAL:HA    | 3:O1:139:SER:CB   | 2.36                     | 0.55              |
| 5:Q1:187:PHE:HA    | 5:Q1:193:VAL:HA   | 1.88                     | 0.55              |
| 6:R1:91:GLU:N      | 6:R1:92:PRO:HD2   | 2.22                     | 0.55              |
| 8:T1:15:ASP:HB2    | 8:T1:16:PRO:CD    | 2.37                     | 0.55              |
| 12:22:68:MET:HE2   | 15:52:37:MET:HE2  | 1.87                     | 0.55              |
| 26:H2:51:ARG:NH1   | 34:Q2:151:ASN:OD1 | 2.40                     | 0.55              |
| 35:R2:203:PRO:HA   | 35:R2:265:PHE:HB2 | 1.88                     | 0.55              |
| 1:A1:109:ALA:O     | 1:A1:112:LEU:N    | 2.40                     | 0.54              |
| 3:C1:378:LYS:HD3   | 6:F1:33:ARG:HH12  | 1.72                     | 0.54              |
| 1:M1:136:GLN:HE21  | 9:U1:50:LEU:HB3   | 1.70                     | 0.54              |
| 1:M1:394:GLU:O     | 1:M1:395:TRP:C    | 2.47                     | 0.54              |
| 1:M1:413:LYS:HB2   | 1:M1:414:TYR:CD2  | 2.42                     | 0.54              |
| 4:P1:94:PRO:HB2    | 4:P1:95:TYR:CE1   | 2.42                     | 0.54              |
| 8:T1:40:CYS:HB2    | 8:T1:57:GLU:HG2   | 1.89                     | 0.54              |
| 17:82:174:ARG:NH2  | 24:F2:87:ASP:O    | 2.40                     | 0.54              |
| 18:92:44:THR:OG1   | 19:A2:209:TYR:HE2 | 1.84                     | 0.54              |
| 19:A2:303:THR:CG2  | 38:U2:136:GLU:CB  | 2.84                     | 0.54              |
| 35:R2:354:ARG:O    | 35:R2:355:ARG:NH2 | 2.36                     | 0.54              |
| 40:W2:91:ASP:H     | 43:Z2:45:TRP:HB3  | 1.71                     | 0.54              |
| 48:f2:32:ILE:O     | 53:62:436:ARG:NH2 | 2.37                     | 0.54              |
| 56:A3:69:MET:HE2   | 56:A3:70:VAL:CG2  | 2.35                     | 0.54              |
| 2:B1:266:SER:O     | 2:B1:269:ALA:HB3  | 2.07                     | 0.54              |
| 3:C1:192:ILE:HD13  | 3:C1:192:ILE:N    | 2.21                     | 0.54              |
| 2:N1:408:ALA:O     | 2:N1:411:ILE:N    | 2.40                     | 0.54              |
| 3:O1:234:LEU:HD21  | 4:P1:216:LEU:CD2  | 2.37                     | 0.54              |
| 4:P1:50:HIS:HE1    | 4:P1:91:PHE:HZ    | 1.54                     | 0.54              |
| 70:P1:301:HEC:HBC2 | 70:P1:301:HEC:CHD | 2.26                     | 0.54              |
| 9:U1:58:GLN:HG2    | 9:U1:78:TYR:HD2   | 1.72                     | 0.54              |
| 19:A2:674:LEU:CD1  | 29:K2:46:LYS:HD2  | 2.37                     | 0.54              |
| 27:I2:106:GLU:O    | 27:I2:108:LYS:HG3 | 2.07                     | 0.54              |
| 52:12:127:TYR:C    | 52:12:127:TYR:CD1 | 2.86                     | 0.54              |
| 58:C3:151:LEU:HB2  | 58:C3:159:MET:HG3 | 1.89                     | 0.54              |
| 1:A1:18:GLN:HG2    | 1:A1:19:LEU:O     | 2.07                     | 0.54              |
| 1:A1:255:ILE:HG13  | 1:A1:422:VAL:CG2  | 2.37                     | 0.54              |
| 3:C1:61:THR:O      | 3:C1:64:SER:N     | 2.41                     | 0.54              |
| 3:C1:68:HIS:NE2    | 5:E1:67:ASP:HB2   | 2.22                     | 0.54              |
| 3:C1:88:SER:O      | 3:C1:89:MET:C     | 2.47                     | 0.54              |
| 3:C1:102:LEU:HB3   | 3:C1:325:PHE:HE1  | 1.71                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:C1:106:SER:O     | 3:C1:109:PHE:CD1  | 2.54                     | 0.54              |
| 3:O1:170:VAL:HG13  | 3:O1:174:THR:CG2  | 2.34                     | 0.54              |
| 4:P1:128:PHE:HB2   | 4:P1:187:CYS:SG   | 2.46                     | 0.54              |
| 7:S1:27:PRO:O      | 7:S1:28:HIS:C     | 2.48                     | 0.54              |
| 10:V1:18:SER:HB3   | 11:W1:23:LEU:HB2  | 1.90                     | 0.54              |
| 19:A2:137:CYS:SG   | 19:A2:138:ASP:N   | 2.80                     | 0.54              |
| 55:e2:136:PHE:O    | 55:e2:140:MET:N   | 2.40                     | 0.54              |
| 58:C3:222:GLN:HE21 | 58:C3:222:GLN:HA  | 1.72                     | 0.54              |
| 64:I3:63:MET:HB3   | 64:I3:68:ILE:HD11 | 1.89                     | 0.54              |
| 1:A1:143:THR:O     | 1:A1:143:THR:CG2  | 2.56                     | 0.54              |
| 1:A1:256:ALA:HA    | 1:A1:320:LEU:O    | 2.06                     | 0.54              |
| 1:A1:343:MET:O     | 1:A1:344:ARG:C    | 2.41                     | 0.54              |
| 2:B1:33:LEU:HB2    | 2:B1:204:MET:O    | 2.07                     | 0.54              |
| 3:C1:25:SER:HA     | 3:C1:218:ILE:HD12 | 1.89                     | 0.54              |
| 3:C1:88:SER:HA     | 3:C1:272:TRP:HZ2  | 1.73                     | 0.54              |
| 3:C1:115:ILE:O     | 3:C1:116:GLY:C    | 2.46                     | 0.54              |
| 4:D1:11:PRO:HB2    | 8:H1:74:PHE:CG    | 2.41                     | 0.54              |
| 4:D1:131:LEU:CD2   | 4:D1:163:PRO:HB3  | 2.38                     | 0.54              |
| 5:E1:29:SER:CA     | 5:E1:32:ARG:HD3   | 2.37                     | 0.54              |
| 6:F1:55:TYR:CD1    | 6:F1:55:TYR:C     | 2.86                     | 0.54              |
| 10:J1:32:GLU:HG2   | 10:J1:33:ARG:N    | 2.22                     | 0.54              |
| 10:J1:51:LEU:HB3   | 10:J1:52:TRP:CE3  | 2.42                     | 0.54              |
| 1:M1:51:LYS:O      | 1:M1:53:ASN:N     | 2.38                     | 0.54              |
| 1:M1:61:HIS:CB     | 1:M1:130:GLU:HG3  | 2.38                     | 0.54              |
| 2:N1:372:VAL:O     | 2:N1:372:VAL:HG12 | 2.08                     | 0.54              |
| 5:Q1:85:LYS:CG     | 5:Q1:86:ASN:H     | 2.12                     | 0.54              |
| 8:T1:68:CYS:O      | 8:T1:69:VAL:C     | 2.51                     | 0.54              |
| 17:82:222:LYS:O    | 25:G2:175:LYS:NZ  | 2.40                     | 0.54              |
| 34:Q2:110:CYS:HA   | 34:Q2:113:ASP:HB3 | 1.88                     | 0.54              |
| 58:C3:156:ARG:HG3  | 58:C3:156:ARG:NH1 | 2.23                     | 0.54              |
| 1:A1:111:GLU:HG2   | 1:A1:213:GLN:HE22 | 1.73                     | 0.54              |
| 1:A1:317:THR:HG22  | 1:A1:318:GLY:N    | 2.21                     | 0.54              |
| 1:A1:334:MET:HA    | 1:A1:334:MET:CE   | 2.37                     | 0.54              |
| 3:C1:124:MET:HG2   | 3:C1:274:PHE:HE1  | 1.71                     | 0.54              |
| 4:D1:51:LEU:HD22   | 4:D1:58:GLU:HA    | 1.89                     | 0.54              |
| 5:E1:63:SER:O      | 5:E1:64:ALA:HB2   | 2.08                     | 0.54              |
| 1:M1:106:LEU:O     | 1:M1:107:PRO:C    | 2.51                     | 0.54              |
| 1:M1:433:ASP:CG    | 3:O1:223:TYR:HH   | 2.13                     | 0.54              |
| 5:Q1:78:LEU:HD21   | 5:Q1:132:TRP:CZ2  | 2.43                     | 0.54              |
| 9:U1:53:GLU:O      | 9:U1:54:SER:C     | 2.51                     | 0.54              |
| 12:22:240:MET:HE1  | 51:j2:48:ILE:HG23 | 1.89                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:A2:650:SER:OG   | 29:K2:56:ARG:HD2  | 2.08                     | 0.54              |
| 20:B2:91:ALA:CB    | 20:B2:193:ASP:OD2 | 2.50                     | 0.54              |
| 49:h2:138:GLU:OE1  | 49:h2:140:ASN:ND2 | 2.41                     | 0.54              |
| 40:M2:35:HIS:H     | 40:M2:39:ASP:HB3  | 1.72                     | 0.54              |
| 61:F3:82:CYS:N     | 61:F3:86:GLY:O    | 2.40                     | 0.54              |
| 1:A1:236:PHE:CD2   | 1:A1:258:GLU:CB   | 2.91                     | 0.54              |
| 1:A1:346:CYS:HB3   | 1:A1:412:SER:HG   | 1.70                     | 0.54              |
| 2:B1:100:SER:HB3   | 2:B1:105:MET:HG3  | 1.88                     | 0.54              |
| 5:E1:52:LYS:NZ     | 10:J1:32:GLU:OE1  | 2.40                     | 0.54              |
| 1:M1:22:GLY:O      | 1:M1:24:ARG:HG2   | 2.08                     | 0.54              |
| 1:M1:241:ILE:HG13  | 7:S1:16:TYR:CE2   | 2.43                     | 0.54              |
| 1:M1:336:PHE:HE2   | 1:M1:446:PHE:HD2  | 1.55                     | 0.54              |
| 2:N1:95:LYS:HE3    | 2:N1:97:SER:OG    | 2.08                     | 0.54              |
| 3:O1:37:LEU:HD11   | 3:O1:97:HIS:CG    | 2.43                     | 0.54              |
| 3:O1:133:LEU:HB2   | 3:O1:134:PRO:HD3  | 1.90                     | 0.54              |
| 4:P1:69:GLU:HG3    | 4:P1:84:PRO:HA    | 1.89                     | 0.54              |
| 17:82:201:ALA:HB1  | 18:92:121:MET:HB2 | 1.90                     | 0.54              |
| 19:A2:272:ARG:NH1  | 25:G2:87:MET:HE3  | 2.23                     | 0.54              |
| 19:A2:381:LEU:HB2  | 29:K2:55:ILE:HD12 | 1.89                     | 0.54              |
| 45:b2:118:SER:OG   | 49:h2:108:TYR:O   | 2.25                     | 0.54              |
| 1:A1:39:VAL:CG2    | 1:A1:197:LEU:HD22 | 2.37                     | 0.54              |
| 1:A1:397:SER:OG    | 1:A1:398:ARG:N    | 2.41                     | 0.54              |
| 1:A1:418:GLN:O     | 1:A1:420:PRO:HD3  | 2.08                     | 0.54              |
| 2:B1:163:LEU:HD22  | 2:B1:256:ALA:HB1  | 1.90                     | 0.54              |
| 3:C1:88:SER:CB     | 3:C1:250:LEU:HD23 | 2.37                     | 0.54              |
| 3:C1:88:SER:HB3    | 3:C1:250:LEU:CD2  | 2.38                     | 0.54              |
| 6:F1:7:SER:HA      | 6:F1:11:ARG:HE    | 1.73                     | 0.54              |
| 6:F1:40:ASN:CG     | 6:F1:41:ASP:H     | 2.16                     | 0.54              |
| 1:M1:324:PHE:CD1   | 1:M1:334:MET:HG2  | 2.42                     | 0.54              |
| 3:O1:76:GLY:HA2    | 3:O1:79:ILE:HD12  | 1.90                     | 0.54              |
| 3:O1:169:SER:OG    | 3:O1:170:VAL:N    | 2.37                     | 0.54              |
| 5:Q1:118:ARG:HH22  | 5:Q1:173:LYS:CA   | 2.20                     | 0.54              |
| 14:42:403:THR:HA   | 14:42:406:TYR:HB3 | 1.90                     | 0.54              |
| 19:A2:111:LYS:CD   | 33:P2:53:TYR:HE2  | 2.20                     | 0.54              |
| 48:f2:150:ARG:HH22 | 55:e2:95:PRO:HB3  | 1.73                     | 0.54              |
| 53:62:361:GLY:O    | 53:62:364:LYS:NZ  | 2.40                     | 0.54              |
| 57:B3:203:ASN:HD22 | 57:B3:206:PHE:HD2 | 1.55                     | 0.54              |
| 59:D3:40:LEU:HD13  | 59:D3:59:LEU:HD13 | 1.90                     | 0.54              |
| 1:A1:61:HIS:CB     | 1:A1:130:GLU:HG3  | 2.37                     | 0.54              |
| 1:A1:173:ASN:O     | 1:A1:177:LEU:HB2  | 2.07                     | 0.54              |
| 2:B1:90:GLU:O      | 2:B1:92:VAL:N     | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:30:TRP:HA     | 3:C1:33:PHE:HE2    | 1.73                     | 0.54              |
| 3:C1:58:ASP:OD2    | 3:O1:56:THR:HG21   | 2.08                     | 0.54              |
| 3:C1:264:THR:O     | 3:C1:266:PRO:HD3   | 2.06                     | 0.54              |
| 3:C1:348:ILE:O     | 3:C1:352:GLN:HG3   | 2.08                     | 0.54              |
| 4:D1:4:GLU:HG3     | 4:D1:6:HIS:CE1     | 2.43                     | 0.54              |
| 1:M1:240:GLN:HA    | 1:M1:422:VAL:O     | 2.06                     | 0.54              |
| 2:N1:88:GLY:O      | 2:N1:91:ALA:HB3    | 2.07                     | 0.54              |
| 4:P1:168:VAL:O     | 4:P1:169:LEU:HD23  | 2.08                     | 0.54              |
| 14:42:319:HIS:HA   | 14:42:322:THR:HB   | 1.89                     | 0.54              |
| 17:82:220:GLN:HE21 | 18:92:118:PHE:HB2  | 1.72                     | 0.54              |
| 19:A2:110:LYS:HD2  | 33:P2:55:CYS:SG    | 2.48                     | 0.54              |
| 48:f2:61:THR:O     | 48:f2:65:ARG:N     | 2.40                     | 0.54              |
| 1:A1:53:ASN:C      | 1:A1:53:ASN:HD22   | 2.16                     | 0.54              |
| 1:A1:89:TYR:CD1    | 1:A1:89:TYR:C      | 2.85                     | 0.54              |
| 1:A1:241:ILE:HG23  | 1:A1:241:ILE:O     | 2.07                     | 0.54              |
| 4:D1:50:HIS:HE1    | 4:D1:91:PHE:HZ     | 1.53                     | 0.54              |
| 1:M1:426:GLY:HA3   | 1:M1:428:ILE:H     | 1.71                     | 0.54              |
| 1:M1:445:ARG:O     | 1:M1:446:PHE:CB    | 2.55                     | 0.54              |
| 2:N1:255:ALA:HB2   | 2:N1:426:ALA:CB    | 2.37                     | 0.54              |
| 2:N1:280:GLY:HA2   | 2:N1:311:ALA:CB    | 2.38                     | 0.54              |
| 3:O1:7:SER:O       | 3:O1:8:HIS:O       | 2.26                     | 0.54              |
| 3:O1:377:LEU:HB3   | 6:R1:33:ARG:HD2    | 1.88                     | 0.54              |
| 4:P1:51:LEU:HD22   | 4:P1:58:GLU:HA     | 1.90                     | 0.54              |
| 4:P1:216:LEU:N     | 4:P1:217:PRO:HD2   | 2.22                     | 0.54              |
| 5:Q1:109:GLU:HG2   | 5:Q1:167:ALA:CB    | 2.25                     | 0.54              |
| 8:T1:35:GLU:O      | 8:T1:39:LEU:HG     | 2.07                     | 0.54              |
| 14:42:289:SER:HB3  | 14:42:406:TYR:HE2  | 1.71                     | 0.54              |
| 27:I2:106:GLU:HB3  | 27:I2:108:LYS:NZ   | 2.23                     | 0.54              |
| 30:L2:59:ASP:HB3   | 34:Q2:130:LYS:HD2  | 1.90                     | 0.54              |
| 34:Q2:9:SER:HA     | 39:V2:88:ARG:HH12  | 1.73                     | 0.54              |
| 57:B3:165:VAL:HB   | 57:B3:170:LEU:HD12 | 1.90                     | 0.54              |
| 2:B1:303:VAL:CG1   | 2:B1:304:HIS:N     | 2.70                     | 0.54              |
| 3:C1:183:PHE:CE1   | 3:C1:187:PHE:CE2   | 2.96                     | 0.54              |
| 6:F1:35:ASP:OD2    | 6:F1:61:ARG:HD2    | 2.07                     | 0.54              |
| 8:H1:73:LEU:HG     | 8:H1:73:LEU:O      | 2.08                     | 0.54              |
| 4:P1:138:PRO:O     | 4:P1:139:THR:C     | 2.50                     | 0.54              |
| 4:P1:220:TYR:HE2   | 7:S1:26:PHE:CE1    | 2.19                     | 0.54              |
| 19:A2:302:LEU:HB3  | 38:U2:137:TRP:HB3  | 1.90                     | 0.54              |
| 23:E2:82:ALA:HB2   | 33:P2:25:GLN:HE21  | 1.73                     | 0.54              |
| 56:A3:398:PRO:O    | 56:A3:498:CYS:HB3  | 2.08                     | 0.54              |
| 57:B3:111:THR:HG21 | 63:H3:66:ILE:HD11  | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:40:TRP:CZ2   | 1:A1:377:GLU:CA   | 2.89                     | 0.53              |
| 2:B1:62:ASN:ND2   | 2:B1:62:ASN:O     | 2.41                     | 0.53              |
| 2:B1:340:ALA:O    | 2:B1:344:VAL:HG23 | 2.08                     | 0.53              |
| 3:C1:309:THR:CG2  | 3:C1:370:GLY:HA3  | 2.38                     | 0.53              |
| 1:M1:88:ALA:O     | 2:N1:286:LYS:HE2  | 2.07                     | 0.53              |
| 2:N1:258:VAL:HG12 | 2:N1:321:LEU:HD22 | 1.89                     | 0.53              |
| 5:Q1:139:CYS:O    | 5:Q1:143:GLY:HA2  | 2.08                     | 0.53              |
| 6:R1:51:PRO:HG2   | 6:R1:54:LEU:HB2   | 1.89                     | 0.53              |
| 20:B2:87:GLN:CB   | 20:B2:89:PRO:HD3  | 2.32                     | 0.53              |
| 61:F3:51:SER:HB2  | 61:F3:91:LEU:HD11 | 1.90                     | 0.53              |
| 1:A1:252:HIS:CD2  | 1:A1:325:VAL:CG2  | 2.92                     | 0.53              |
| 2:B1:160:ILE:HD11 | 2:B1:325:TYR:HE2  | 1.74                     | 0.53              |
| 2:B1:262:ALA:HB2  | 2:B1:272:PHE:HE2  | 1.72                     | 0.53              |
| 2:B1:304:HIS:CG   | 2:B1:305:GLN:N    | 2.76                     | 0.53              |
| 2:B1:396:SER:O    | 2:B1:399:LEU:HB2  | 2.08                     | 0.53              |
| 8:H1:66:ASP:O     | 8:H1:67:HIS:C     | 2.50                     | 0.53              |
| 1:M1:204:GLU:HG2  | 1:M1:206:ARG:HB3  | 1.90                     | 0.53              |
| 1:M1:236:PHE:CD2  | 1:M1:258:GLU:CB   | 2.91                     | 0.53              |
| 2:N1:168:TYR:HD2  | 2:N1:238:LYS:O    | 1.92                     | 0.53              |
| 3:O1:207:ASN:ND2  | 3:O1:209:THR:OG1  | 2.41                     | 0.53              |
| 3:O1:265:PRO:O    | 3:O1:268:ILE:HG13 | 2.07                     | 0.53              |
| 4:P1:11:PRO:HB2   | 8:T1:74:PHE:CG    | 2.44                     | 0.53              |
| 4:P1:48:TYR:OH    | 4:P1:68:VAL:HG11  | 2.08                     | 0.53              |
| 5:Q1:32:ARG:HH12  | 7:S1:22:GLU:CD    | 2.15                     | 0.53              |
| 8:T1:70:ALA:HA    | 8:T1:73:LEU:HD22  | 1.89                     | 0.53              |
| 19:A2:311:LYS:HB3 | 38:U2:142:THR:O   | 2.07                     | 0.53              |
| 21:C2:70:ILE:HG13 | 21:C2:71:LEU:HD12 | 1.90                     | 0.53              |
| 59:D3:108:PRO:HG2 | 59:D3:111:PHE:CE2 | 2.42                     | 0.53              |
| 2:B1:140:LEU:HD12 | 2:B1:143:GLN:CB   | 2.38                     | 0.53              |
| 3:C1:1:MET:SD     | 3:C1:4:ILE:HB     | 2.48                     | 0.53              |
| 3:C1:141:TRP:HB3  | 3:C1:268:ILE:HD13 | 1.90                     | 0.53              |
| 4:D1:33:TYR:HA    | 4:D1:37:CYS:HB2   | 1.89                     | 0.53              |
| 5:E1:15:ARG:HH21  | 5:E1:32:ARG:HG3   | 1.74                     | 0.53              |
| 5:E1:20:ASP:O     | 5:E1:21:SER:C     | 2.49                     | 0.53              |
| 10:J1:52:TRP:CE3  | 10:J1:52:TRP:N    | 2.77                     | 0.53              |
| 2:N1:159:VAL:HG12 | 2:N1:160:ILE:N    | 2.21                     | 0.53              |
| 4:P1:237:TYR:HD1  | 7:S1:13:VAL:HG22  | 1.73                     | 0.53              |
| 6:R1:7:SER:HA     | 6:R1:11:ARG:HE    | 1.73                     | 0.53              |
| 52:12:37:PRO:HB2  | 52:12:44:GLY:HA2  | 1.90                     | 0.53              |
| 6:F1:35:ASP:OD1   | 6:F1:89:TYR:OH    | 2.21                     | 0.53              |
| 1:M1:152:TYR:O    | 1:M1:153:LEU:C    | 2.47                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:O1:218:ILE:HD13 | 4:P1:230:LEU:HD13  | 1.91                     | 0.53              |
| 3:O1:251:GLY:O    | 3:O1:252:ASP:C     | 2.51                     | 0.53              |
| 4:P1:106:ASN:C    | 4:P1:106:ASN:HD22  | 2.17                     | 0.53              |
| 5:Q1:171:ILE:HD12 | 5:Q1:176:ALA:HB3   | 1.90                     | 0.53              |
| 8:T1:73:LEU:HD21  | 8:T1:74:PHE:CD1    | 2.43                     | 0.53              |
| 10:V1:49:GLY:HA2  | 10:V1:54:HIS:CB    | 2.39                     | 0.53              |
| 12:22:224:THR:H   | 12:22:228:LEU:HD23 | 1.72                     | 0.53              |
| 15:52:17:VAL:HG12 | 53:62:588:PHE:HB3  | 1.91                     | 0.53              |
| 18:92:111:ARG:NE  | 25:G2:174:THR:OG1  | 2.42                     | 0.53              |
| 19:A2:129:PRO:HG2 | 27:I2:114:TYR:CE1  | 2.43                     | 0.53              |
| 59:D3:52:SER:OG   | 59:D3:55:GLU:HG3   | 2.08                     | 0.53              |
| 61:F3:48:LEU:O    | 61:F3:50:PRO:HD3   | 2.08                     | 0.53              |
| 1:A1:32:GLN:CG    | 1:A1:33:PRO:CD     | 2.86                     | 0.53              |
| 1:A1:106:LEU:HD21 | 1:A1:203:LEU:HD13  | 1.89                     | 0.53              |
| 2:B1:276:GLN:O    | 2:B1:280:GLY:N     | 2.40                     | 0.53              |
| 3:C1:219:PRO:CB   | 3:C1:222:PRO:HD2   | 2.39                     | 0.53              |
| 4:D1:149:PHE:HZ   | 8:H1:55:THR:HG23   | 1.73                     | 0.53              |
| 4:D1:190:LEU:O    | 4:D1:191:ARG:C     | 2.52                     | 0.53              |
| 4:D1:213:GLY:O    | 4:D1:217:PRO:HG3   | 2.07                     | 0.53              |
| 6:F1:16:ILE:O     | 6:F1:17:ARG:C      | 2.50                     | 0.53              |
| 1:M1:25:VAL:HG21  | 1:M1:209:LEU:CD1   | 2.39                     | 0.53              |
| 1:M1:106:LEU:HD22 | 1:M1:203:LEU:CD2   | 2.35                     | 0.53              |
| 2:N1:132:PHE:HD2  | 2:N1:191:LEU:HD13  | 1.67                     | 0.53              |
| 2:N1:285:VAL:HG12 | 2:N1:288:GLY:HA3   | 1.91                     | 0.53              |
| 3:O1:26:ASN:HD22  | 3:O1:208:PRO:HD2   | 1.70                     | 0.53              |
| 3:O1:218:ILE:HG23 | 3:O1:223:TYR:CD2   | 2.43                     | 0.53              |
| 5:Q1:150:ALA:HB3  | 5:Q1:157:TYR:HB3   | 1.91                     | 0.53              |
| 14:42:118:PHE:O   | 14:42:122:PHE:N    | 2.39                     | 0.53              |
| 18:92:95:ILE:HD13 | 19:A2:210:ILE:HG22 | 1.88                     | 0.53              |
| 34:Q2:30:HIS:NE2  | 34:Q2:120:PRO:O    | 2.41                     | 0.53              |
| 46:c2:34:VAL:HG22 | 46:c2:36:PRO:HA    | 1.91                     | 0.53              |
| 1:A1:61:HIS:CD2   | 2:B1:287:ARG:HD3   | 2.43                     | 0.53              |
| 1:A1:134:ILE:HD13 | 1:A1:134:ILE:N     | 2.23                     | 0.53              |
| 1:A1:134:ILE:HA   | 1:A1:137:GLU:HG3   | 1.91                     | 0.53              |
| 2:B1:92:VAL:HG12  | 2:B1:92:VAL:O      | 2.08                     | 0.53              |
| 3:C1:103:TYR:O    | 3:C1:315:MET:CB    | 2.57                     | 0.53              |
| 7:G1:15:THR:HG22  | 7:G1:15:THR:O      | 2.07                     | 0.53              |
| 7:G1:64:GLN:O     | 7:G1:65:GLU:C      | 2.50                     | 0.53              |
| 9:I1:58:GLN:HG2   | 9:I1:78:TYR:HD2    | 1.72                     | 0.53              |
| 10:J1:45:HIS:O    | 10:J1:48:GLU:HG2   | 2.08                     | 0.53              |
| 1:M1:53:ASN:HB3   | 1:M1:170:PRO:CD    | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M1:411:CYS:O    | 1:M1:415:PHE:HD1  | 1.92                     | 0.53              |
| 1:M1:417:ASP:CG   | 10:V1:10:TYR:OH   | 2.51                     | 0.53              |
| 2:N1:133:ARG:O    | 2:N1:134:ARG:C    | 2.49                     | 0.53              |
| 2:N1:276:GLN:O    | 2:N1:280:GLY:N    | 2.40                     | 0.53              |
| 5:Q1:95:PRO:HG2   | 5:Q1:145:VAL:CG2  | 2.38                     | 0.53              |
| 28:J2:64:LYS:H    | 34:Q2:21:SER:HB3  | 1.74                     | 0.53              |
| 50:i2:59:ILE:HA   | 50:i2:62:HIS:HB3  | 1.90                     | 0.53              |
| 57:B3:102:HIS:O   | 57:B3:104:TRP:N   | 2.42                     | 0.53              |
| 59:D3:67:SER:OG   | 59:D3:70:GLU:HG3  | 2.08                     | 0.53              |
| 62:G3:8:HIS:O     | 62:G3:10:GLY:N    | 2.42                     | 0.53              |
| 2:B1:79:GLY:H     | 2:B1:125:ASN:ND2  | 2.07                     | 0.53              |
| 1:M1:29:GLN:HG3   | 1:M1:203:LEU:O    | 2.09                     | 0.53              |
| 1:M1:53:ASN:HB3   | 1:M1:170:PRO:HD2  | 1.89                     | 0.53              |
| 2:N1:25:GLU:O     | 2:N1:213:HIS:CE1  | 2.62                     | 0.53              |
| 2:N1:217:LYS:O    | 2:N1:218:GLN:C    | 2.51                     | 0.53              |
| 2:N1:247:GLN:HG3  | 2:N1:248:ASN:N    | 2.24                     | 0.53              |
| 2:N1:262:ALA:HB3  | 2:N1:269:ALA:HA   | 1.91                     | 0.53              |
| 3:O1:71:ARG:NH2   | 4:P1:193:ALA:O    | 2.42                     | 0.53              |
| 3:O1:345:HIS:CB   | 3:O1:346:PRO:HD3  | 2.26                     | 0.53              |
| 4:P1:219:VAL:HA   | 4:P1:222:MET:HG3  | 1.89                     | 0.53              |
| 4:P1:237:TYR:CE2  | 4:P1:239:PRO:HG3  | 2.44                     | 0.53              |
| 19:A2:637:ASP:OD1 | 32:O2:118:PHE:CE1 | 2.62                     | 0.53              |
| 49:h2:81:ALA:O    | 49:h2:83:ASP:N    | 2.42                     | 0.53              |
| 56:A3:268:PHE:CZ  | 57:B3:58:ALA:HA   | 2.44                     | 0.53              |
| 60:E3:41:LEU:HD12 | 60:E3:41:LEU:O    | 2.08                     | 0.53              |
| 61:F3:55:LYS:HA   | 61:F3:74:LEU:O    | 2.08                     | 0.53              |
| 1:A1:162:PRO:O    | 1:A1:165:GLN:NE2  | 2.38                     | 0.53              |
| 2:B1:316:TYR:OH   | 9:I1:64:LEU:HD23  | 2.09                     | 0.53              |
| 3:O1:219:PRO:HB2  | 3:O1:222:PRO:HD2  | 1.89                     | 0.53              |
| 3:O1:276:PHE:O    | 3:O1:277:ALA:C    | 2.52                     | 0.53              |
| 4:P1:3:LEU:HD21   | 7:S1:71:ARG:HA    | 1.90                     | 0.53              |
| 4:P1:69:GLU:O     | 4:P1:73:GLY:HA3   | 2.09                     | 0.53              |
| 19:A2:134:GLY:O   | 20:B2:382:PHE:HE2 | 1.92                     | 0.53              |
| 19:A2:238:PHE:HE2 | 23:E2:138:GLY:O   | 1.92                     | 0.53              |
| 59:D3:23:PRO:HD2  | 60:E3:34:ASN:HD22 | 1.74                     | 0.53              |
| 1:A1:34:THR:HB    | 2:B1:373:GLU:OE1  | 2.09                     | 0.53              |
| 4:D1:138:PRO:HG2  | 8:H1:55:THR:CB    | 2.38                     | 0.53              |
| 5:E1:2:HIS:O      | 5:E1:5:ILE:HG12   | 2.09                     | 0.53              |
| 6:F1:25:GLY:O     | 6:F1:28:LYS:HG3   | 2.09                     | 0.53              |
| 1:M1:106:LEU:HB3  | 1:M1:107:PRO:HD3  | 1.90                     | 0.53              |
| 2:N1:294:SER:O    | 2:N1:295:LEU:C    | 2.51                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:P1:120:ARG:HG2   | 4:P1:120:ARG:NH1   | 2.24                     | 0.53              |
| 5:Q1:45:VAL:CG2    | 10:V1:24:ILE:HA    | 2.39                     | 0.53              |
| 6:R1:75:LEU:CD1    | 6:R1:76:PRO:HD2    | 2.36                     | 0.53              |
| 17:82:415:ILE:HD12 | 19:A2:119:PHE:HE1  | 1.72                     | 0.53              |
| 19:A2:301:ARG:O    | 38:U2:137:TRP:N    | 2.41                     | 0.53              |
| 54:g2:14:PRO:O     | 54:g2:116:ARG:NH2  | 2.42                     | 0.53              |
| 57:B3:136:LEU:HB3  | 57:B3:193:TYR:HD2  | 1.73                     | 0.53              |
| 1:A1:85:HIS:HA     | 2:B1:284:HIS:O     | 2.09                     | 0.53              |
| 2:B1:300:ALA:HA    | 2:B1:307:PHE:HZ    | 1.74                     | 0.53              |
| 3:C1:90:PHE:CE1    | 3:C1:123:VAL:HG21  | 2.44                     | 0.53              |
| 8:H1:65:ARG:HG3    | 8:H1:66:ASP:N      | 2.23                     | 0.53              |
| 10:J1:52:TRP:HE3   | 10:J1:52:TRP:H     | 1.57                     | 0.53              |
| 10:J1:56:LYS:HE2   | 10:J1:60:GLU:OE1   | 2.09                     | 0.53              |
| 1:M1:317:THR:HG22  | 1:M1:318:GLY:H     | 1.73                     | 0.53              |
| 2:N1:262:ALA:HB2   | 2:N1:268:GLU:HB3   | 1.90                     | 0.53              |
| 3:O1:106:SER:O     | 3:O1:109:PHE:CD2   | 2.54                     | 0.53              |
| 3:O1:174:THR:O     | 3:O1:178:PHE:CD2   | 2.62                     | 0.53              |
| 3:O1:196:HIS:CE1   | 69:O1:402:HEM:C1D  | 2.97                     | 0.53              |
| 10:V1:4:THR:HG22   | 10:V1:6:THR:OG1    | 2.09                     | 0.53              |
| 19:A2:473:MET:HE2  | 19:A2:475:ILE:HD11 | 1.91                     | 0.53              |
| 40:W2:83:VAL:HG21  | 40:W2:145:VAL:HG22 | 1.91                     | 0.53              |
| 56:A3:11:ASN:ND2   | 56:A3:14:ASP:H     | 2.07                     | 0.53              |
| 1:A1:11:VAL:CG1    | 1:A1:12:PRO:HD2    | 2.39                     | 0.52              |
| 1:A1:67:THR:OG1    | 1:A1:119:ASN:HB2   | 2.09                     | 0.52              |
| 2:B1:132:PHE:CD2   | 2:B1:191:LEU:HD13  | 2.43                     | 0.52              |
| 2:B1:160:ILE:CD1   | 2:B1:325:TYR:HE2   | 2.21                     | 0.52              |
| 2:B1:347:ILE:H     | 2:B1:347:ILE:CD1   | 2.21                     | 0.52              |
| 2:B1:435:PHE:CE1   | 2:N1:169:ARG:HG2   | 2.44                     | 0.52              |
| 3:C1:80:ARG:O      | 3:C1:80:ARG:HD3    | 2.09                     | 0.52              |
| 3:C1:103:TYR:HA    | 3:C1:315:MET:CE    | 2.32                     | 0.52              |
| 4:D1:48:TYR:OH     | 4:D1:68:VAL:HG11   | 2.09                     | 0.52              |
| 7:G1:25:ALA:O      | 7:G1:27:PRO:HD3    | 2.09                     | 0.52              |
| 2:N1:277:HIS:CD2   | 2:N1:364:LEU:HD13  | 2.43                     | 0.52              |
| 2:N1:406:ALA:HB3   | 2:N1:409:ASP:HB2   | 1.92                     | 0.52              |
| 4:P1:27:ARG:O      | 4:P1:28:ARG:C      | 2.52                     | 0.52              |
| 4:P1:181:GLN:HG2   | 8:T1:77:LEU:CD2    | 2.21                     | 0.52              |
| 4:P1:237:TYR:CE2   | 4:P1:239:PRO:HD3   | 2.44                     | 0.52              |
| 8:T1:58:LEU:HD12   | 8:T1:58:LEU:O      | 2.10                     | 0.52              |
| 10:V1:36:ASP:O     | 10:V1:37:GLN:C     | 2.53                     | 0.52              |
| 12:22:164:ILE:HG13 | 53:62:576:LEU:HD11 | 1.89                     | 0.52              |
| 14:42:439:LEU:H    | 14:42:442:LEU:HD13 | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:52:93:LEU:HD22  | 53:62:583:LEU:H    | 1.73                     | 0.52              |
| 21:C2:170:ARG:HG3  | 21:C2:186:LEU:HD12 | 1.91                     | 0.52              |
| 57:B3:68:LEU:HB3   | 57:B3:69:PRO:HD3   | 1.91                     | 0.52              |
| 62:G3:2:SER:OG     | 62:G3:3:ALA:N      | 2.41                     | 0.52              |
| 2:B1:69:LEU:HD21   | 2:B1:199:PHE:CZ    | 2.44                     | 0.52              |
| 2:B1:141:GLN:OE1   | 2:B1:183:ILE:O     | 2.27                     | 0.52              |
| 2:B1:268:GLU:O     | 2:B1:271:ALA:HB3   | 2.10                     | 0.52              |
| 4:D1:82:MET:HE2    | 4:D1:86:LYS:NZ     | 2.23                     | 0.52              |
| 8:H1:73:LEU:CD2    | 8:H1:74:PHE:HD1    | 2.21                     | 0.52              |
| 1:M1:64:PHE:HE1    | 1:M1:86:LEU:CG     | 2.22                     | 0.52              |
| 1:M1:244:ARG:CZ    | 7:S1:10:VAL:HB     | 2.38                     | 0.52              |
| 1:M1:408:ARG:NH2   | 11:W1:15:ARG:CZ    | 2.65                     | 0.52              |
| 3:O1:174:THR:O     | 3:O1:178:PHE:HD2   | 1.90                     | 0.52              |
| 3:O1:200:LEU:HD13  | 69:O1:402:HEM:HAD2 | 1.90                     | 0.52              |
| 3:O1:275:LEU:O     | 3:O1:278:TYR:N     | 2.42                     | 0.52              |
| 5:Q1:81:ILE:H      | 5:Q1:81:ILE:HD12   | 1.75                     | 0.52              |
| 6:R1:96:GLU:OE2    | 6:R1:99:ARG:NH1    | 2.43                     | 0.52              |
| 12:22:196:TYR:OH   | 37:T2:137:ALA:O    | 2.26                     | 0.52              |
| 19:A2:313:LEU:CG   | 38:U2:142:THR:CA   | 2.86                     | 0.52              |
| 36:S2:32:ILE:HG13  | 36:S2:33:LEU:HD12  | 1.92                     | 0.52              |
| 53:62:241:THR:HG23 | 53:62:299:LYS:HZ1  | 1.74                     | 0.52              |
| 53:62:427:ILE:HG13 | 53:62:431:LEU:HD12 | 1.91                     | 0.52              |
| 59:D3:128:VAL:O    | 59:D3:134:PHE:HB3  | 2.09                     | 0.52              |
| 63:H3:75:ARG:HG2   | 63:H3:75:ARG:NH1   | 2.19                     | 0.52              |
| 1:A1:53:ASN:CG     | 1:A1:165:GLN:HB2   | 2.34                     | 0.52              |
| 3:C1:92:ILE:O      | 3:C1:96:MET:HG2    | 2.09                     | 0.52              |
| 5:E1:31:ALA:O      | 5:E1:34:GLY:N      | 2.42                     | 0.52              |
| 6:F1:45:GLU:O      | 6:F1:49:ARG:HG3    | 2.08                     | 0.52              |
| 1:M1:277:ILE:CG2   | 1:M1:294:LEU:HD12  | 2.39                     | 0.52              |
| 3:O1:304:ILE:N     | 3:O1:305:PRO:CD    | 2.72                     | 0.52              |
| 4:P1:11:PRO:HG2    | 8:T1:74:PHE:HB2    | 1.92                     | 0.52              |
| 19:A2:126:LEU:HB2  | 27:I2:98:ARG:O     | 2.10                     | 0.52              |
| 53:62:550:SER:OG   | 53:62:551:SER:N    | 2.42                     | 0.52              |
| 56:A3:302:ARG:O    | 56:A3:306:THR:HG23 | 2.09                     | 0.52              |
| 1:A1:239:SER:OG    | 1:A1:240:GLN:N     | 2.39                     | 0.52              |
| 1:A1:260:PRO:HD3   | 1:A1:414:TYR:CD1   | 2.44                     | 0.52              |
| 2:B1:135:TRP:CD1   | 2:B1:136:GLU:HG3   | 2.44                     | 0.52              |
| 2:B1:191:LEU:O     | 2:B1:195:VAL:HG23  | 2.09                     | 0.52              |
| 3:C1:103:TYR:O     | 3:C1:315:MET:HB2   | 2.10                     | 0.52              |
| 3:C1:135:TRP:CH2   | 3:C1:170:VAL:O     | 2.62                     | 0.52              |
| 3:C1:301:LEU:HA    | 3:C1:304:ILE:HD12  | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:350:ILE:O     | 3:C1:351:GLY:C     | 2.53                     | 0.52              |
| 3:C1:368:THR:O     | 3:C1:371:THR:HB    | 2.10                     | 0.52              |
| 1:M1:25:VAL:HG21   | 1:M1:209:LEU:HD13  | 1.91                     | 0.52              |
| 1:M1:41:ILE:HD12   | 1:M1:41:ILE:N      | 2.24                     | 0.52              |
| 1:M1:277:ILE:HB    | 1:M1:309:THR:HG21  | 1.91                     | 0.52              |
| 2:N1:164:HIS:O     | 2:N1:173:ALA:HA    | 2.09                     | 0.52              |
| 3:O1:218:ILE:HG21  | 3:O1:223:TYR:CD2   | 2.43                     | 0.52              |
| 6:R1:75:LEU:C      | 6:R1:80:TRP:HE1    | 2.17                     | 0.52              |
| 19:A2:157:LYS:HB2  | 27:I2:100:TYR:HE2  | 1.71                     | 0.52              |
| 20:B2:86:PRO:HG3   | 20:B2:96:ARG:HB3   | 1.90                     | 0.52              |
| 61:F3:8:THR:OG1    | 61:F3:11:GLU:HG2   | 2.10                     | 0.52              |
| 2:B1:122:PHE:O     | 2:B1:123:LEU:C     | 2.53                     | 0.52              |
| 2:B1:308:ASP:OD2   | 9:I1:55:LEU:HA     | 2.10                     | 0.52              |
| 3:C1:119:LEU:HD23  | 69:C1:402:HEM:C4B  | 2.44                     | 0.52              |
| 4:D1:68:VAL:HG12   | 4:D1:92:PRO:HG2    | 1.91                     | 0.52              |
| 4:D1:233:ARG:HG3   | 7:G1:17:SER:CB     | 2.40                     | 0.52              |
| 5:E1:18:VAL:HG11   | 5:E1:32:ARG:HH11   | 1.73                     | 0.52              |
| 9:I1:58:GLN:HB3    | 9:I1:78:TYR:HB2    | 1.91                     | 0.52              |
| 1:M1:111:GLU:HG2   | 1:M1:213:GLN:NE2   | 2.25                     | 0.52              |
| 1:M1:241:ILE:CD1   | 7:S1:16:TYR:CE2    | 2.92                     | 0.52              |
| 1:M1:292:SER:O     | 1:M1:295:ALA:HB3   | 2.09                     | 0.52              |
| 2:N1:304:HIS:CD2   | 2:N1:305:GLN:N     | 2.78                     | 0.52              |
| 4:P1:146:GLY:O     | 4:P1:148:TYR:N     | 2.42                     | 0.52              |
| 4:P1:195:GLU:HG3   | 4:P1:198:HIS:HB2   | 1.92                     | 0.52              |
| 6:R1:73:GLN:HE21   | 7:S1:32:LYS:HE3    | 1.74                     | 0.52              |
| 8:T1:62:LEU:O      | 8:T1:65:ARG:HG2    | 2.09                     | 0.52              |
| 8:T1:65:ARG:CG     | 8:T1:66:ASP:N      | 2.72                     | 0.52              |
| 14:42:23:ILE:HG21  | 14:42:93:LYS:HE3   | 1.89                     | 0.52              |
| 36:S2:275:ASN:O    | 36:S2:277:ARG:N    | 2.41                     | 0.52              |
| 1:A1:166:SER:CB    | 5:E1:3:THR:HG22    | 2.39                     | 0.52              |
| 2:B1:68:LEU:C      | 2:B1:68:LEU:HD12   | 2.34                     | 0.52              |
| 3:C1:221:HIS:HA    | 3:C1:225:THR:HG23  | 1.92                     | 0.52              |
| 3:C1:377:LEU:O     | 3:C1:378:LYS:HB3   | 2.09                     | 0.52              |
| 5:E1:47:VAL:O      | 5:E1:50:ALA:HB3    | 2.10                     | 0.52              |
| 2:N1:198:HIS:CE1   | 2:N1:233:SER:HB3   | 2.45                     | 0.52              |
| 2:N1:247:GLN:NE2   | 2:N1:429:ASN:HA    | 2.25                     | 0.52              |
| 2:N1:275:LEU:HB2   | 2:N1:410:VAL:HG13  | 1.92                     | 0.52              |
| 3:O1:47:THR:HG22   | 3:O1:83:HIS:HB2    | 1.91                     | 0.52              |
| 5:Q1:102:THR:H     | 5:Q1:105:GLU:HB2   | 1.74                     | 0.52              |
| 6:R1:95:LYS:O      | 6:R1:96:GLU:C      | 2.53                     | 0.52              |
| 12:22:142:LEU:HD23 | 12:22:145:ILE:HD12 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:D2:114:ARG:HG3 | 22:D2:114:ARG:NH2  | 2.15                     | 0.52              |
| 23:E2:116:CYS:HA  | 23:E2:140:ARG:HH22 | 1.75                     | 0.52              |
| 35:R2:264:ALA:H   | 35:R2:334:GLY:HA3  | 1.75                     | 0.52              |
| 1:A1:37:VAL:HG13  | 1:A1:199:ALA:CB    | 2.40                     | 0.52              |
| 1:A1:85:HIS:CD2   | 2:B1:370:MET:HE1   | 2.45                     | 0.52              |
| 1:A1:426:GLY:H    | 1:A1:428:ILE:CD1   | 2.22                     | 0.52              |
| 3:C1:85:ASN:O     | 3:C1:86:GLY:C      | 2.50                     | 0.52              |
| 3:C1:183:PHE:CD1  | 3:C1:183:PHE:C     | 2.88                     | 0.52              |
| 3:C1:183:PHE:CD1  | 3:O1:183:PHE:CD1   | 2.97                     | 0.52              |
| 4:D1:79:GLU:HB3   | 4:D1:82:MET:HB2    | 1.91                     | 0.52              |
| 1:M1:426:GLY:HA2  | 1:M1:428:ILE:CG1   | 2.37                     | 0.52              |
| 3:O1:27:ILE:O     | 3:O1:27:ILE:CG2    | 2.58                     | 0.52              |
| 3:O1:296:PHE:O    | 3:O1:297:SER:C     | 2.52                     | 0.52              |
| 4:P1:55:CYS:SG    | 10:V1:52:TRP:CB    | 2.97                     | 0.52              |
| 4:P1:138:PRO:HB3  | 8:T1:55:THR:HA     | 1.90                     | 0.52              |
| 19:A2:314:LEU:CD2 | 38:U2:140:PRO:CD   | 2.69                     | 0.52              |
| 20:B2:299:GLN:HG2 | 23:E2:38:TYR:HE1   | 1.75                     | 0.52              |
| 57:B3:33:LEU:HD23 | 64:I3:28:SER:HB2   | 1.91                     | 0.52              |
| 60:E3:63:SER:O    | 60:E3:67:ILE:HG13  | 2.10                     | 0.52              |
| 2:B1:257:LEU:HD13 | 2:B1:424:MET:HE2   | 1.91                     | 0.52              |
| 4:D1:10:TYR:HD1   | 8:H1:74:PHE:CE1    | 2.28                     | 0.52              |
| 4:D1:64:LEU:O     | 4:D1:68:VAL:HG23   | 2.09                     | 0.52              |
| 4:D1:139:THR:HG21 | 8:H1:41:ASP:O      | 2.09                     | 0.52              |
| 7:G1:33:GLY:O     | 7:G1:37:VAL:N      | 2.36                     | 0.52              |
| 1:M1:5:ALA:O      | 1:M1:6:GLN:C       | 2.53                     | 0.52              |
| 1:M1:151:ASN:O    | 1:M1:152:TYR:C     | 2.53                     | 0.52              |
| 1:M1:392:LEU:HA   | 1:M1:395:TRP:NE1   | 2.25                     | 0.52              |
| 2:N1:262:ALA:HB3  | 2:N1:269:ALA:N     | 2.24                     | 0.52              |
| 3:O1:246:ALA:N    | 3:O1:247:PRO:CD    | 2.73                     | 0.52              |
| 5:Q1:76:ILE:CG2   | 5:Q1:194:ILE:CG1   | 2.74                     | 0.52              |
| 12:22:87:MET:HE3  | 12:22:90:PHE:HE2   | 1.74                     | 0.52              |
| 17:82:390:ASP:OD2 | 19:A2:202:ASN:CB   | 2.51                     | 0.52              |
| 18:92:62:ARG:NH2  | 24:F2:83:TYR:OH    | 2.40                     | 0.52              |
| 35:R2:197:GLU:HB2 | 35:R2:259:ARG:HE   | 1.75                     | 0.52              |
| 52:12:25:ARG:NH1  | 52:12:25:ARG:CG    | 2.73                     | 0.52              |
| 53:62:258:PHE:HA  | 53:62:261:ILE:HD12 | 1.92                     | 0.52              |
| 56:A3:225:GLY:HA3 | 58:C3:112:LEU:HD13 | 1.92                     | 0.52              |
| 57:B3:104:TRP:CG  | 57:B3:203:ASN:HB2  | 2.44                     | 0.52              |
| 1:A1:19:LEU:HB2   | 1:A1:23:LEU:HB3    | 1.92                     | 0.52              |
| 1:A1:91:THR:HG23  | 1:A1:92:ARG:H      | 1.74                     | 0.52              |
| 1:A1:436:ARG:HE   | 3:C1:222:PRO:HG3   | 1.73                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B1:280:GLY:HA2   | 2:B1:311:ALA:CB    | 2.40                     | 0.52              |
| 3:C1:300:ILE:HD13  | 3:C1:362:ILE:HG21  | 1.92                     | 0.52              |
| 4:D1:143:LEU:HD22  | 4:D1:147:LEU:O     | 2.09                     | 0.52              |
| 5:E1:38:LEU:HD13   | 10:J1:9:LEU:HD23   | 1.92                     | 0.52              |
| 6:F1:96:GLU:OE1    | 6:F1:96:GLU:HA     | 2.09                     | 0.52              |
| 1:M1:262:TRP:CE3   | 1:M1:385:THR:CG2   | 2.93                     | 0.52              |
| 2:N1:51:ILE:CG2    | 2:N1:199:PHE:HA    | 2.33                     | 0.52              |
| 2:N1:395:PRO:O     | 2:N1:396:SER:C     | 2.52                     | 0.52              |
| 3:O1:6:LYS:HE2     | 3:O1:16:ASN:HD21   | 1.74                     | 0.52              |
| 3:O1:245:PHE:CG    | 4:P1:17:LEU:HD13   | 2.43                     | 0.52              |
| 22:D2:82:LEU:HB2   | 22:D2:111:VAL:HG22 | 1.90                     | 0.52              |
| 57:B3:100:MET:CE   | 57:B3:157:GLU:HG3  | 2.40                     | 0.52              |
| 1:A1:326:CYS:SG    | 1:A1:331:ILE:HA    | 2.50                     | 0.52              |
| 1:A1:433:ASP:CB    | 3:C1:219:PRO:HG2   | 2.40                     | 0.52              |
| 2:B1:25:GLU:O      | 2:B1:213:HIS:CE1   | 2.63                     | 0.52              |
| 2:B1:97:SER:OG     | 9:I1:70:LEU:HB2    | 2.10                     | 0.52              |
| 4:D1:7:PRO:HB2     | 4:D1:125:ASP:HB3   | 1.92                     | 0.52              |
| 8:H1:15:ASP:N      | 8:H1:16:PRO:CD     | 2.73                     | 0.52              |
| 1:M1:19:LEU:HD13   | 1:M1:214:LYS:HG2   | 1.92                     | 0.52              |
| 1:M1:426:GLY:HA3   | 1:M1:428:ILE:N     | 2.24                     | 0.52              |
| 3:O1:52:ALA:HB2    | 69:O1:401:HEM:CMD  | 2.40                     | 0.52              |
| 3:O1:200:LEU:HD13  | 69:O1:402:HEM:CAD  | 2.40                     | 0.52              |
| 4:P1:160:MET:HE3   | 4:P1:163:PRO:HG3   | 1.91                     | 0.52              |
| 18:92:222:ARG:HD3  | 18:92:228:ALA:HB2  | 1.92                     | 0.52              |
| 35:R2:127:ILE:HG22 | 35:R2:165:ILE:HB   | 1.91                     | 0.52              |
| 2:B1:79:GLY:HA3    | 2:B1:125:ASN:HD21  | 1.75                     | 0.51              |
| 2:B1:279:LEU:HD22  | 2:B1:344:VAL:HG22  | 1.91                     | 0.51              |
| 2:B1:286:LYS:O     | 2:B1:287:ARG:HB2   | 2.09                     | 0.51              |
| 4:D1:62:LYS:O      | 4:D1:66:GLU:HG3    | 2.10                     | 0.51              |
| 6:F1:13:LEU:O      | 6:F1:16:ILE:N      | 2.42                     | 0.51              |
| 3:O1:170:VAL:HG12  | 3:O1:170:VAL:O     | 2.08                     | 0.51              |
| 3:O1:200:LEU:CD1   | 69:O1:402:HEM:HAD2 | 2.40                     | 0.51              |
| 5:Q1:42:THR:O      | 5:Q1:43:THR:C      | 2.53                     | 0.51              |
| 6:R1:46:ALA:O      | 6:R1:47:ILE:C      | 2.53                     | 0.51              |
| 7:S1:67:GLU:O      | 7:S1:71:ARG:HB3    | 2.10                     | 0.51              |
| 8:T1:50:THR:HG22   | 8:T1:51:GLU:N      | 2.25                     | 0.51              |
| 19:A2:674:LEU:CD1  | 29:K2:46:LYS:CD    | 2.88                     | 0.51              |
| 20:B2:97:LEU:HB3   | 20:B2:111:PRO:HB3  | 1.90                     | 0.51              |
| 20:B2:303:ARG:HD3  | 20:B2:401:GLU:HG2  | 1.92                     | 0.51              |
| 21:C2:124:ARG:NH1  | 31:N2:111:GLN:O    | 2.43                     | 0.51              |
| 22:D2:159:GLY:O    | 22:D2:164:HIS:ND1  | 2.42                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:B3:186:SER:CB  | 57:B3:213:LEU:HD22 | 2.40                     | 0.51              |
| 1:A1:34:THR:CB    | 2:B1:373:GLU:OE1   | 2.59                     | 0.51              |
| 1:A1:111:GLU:HG2  | 1:A1:213:GLN:NE2   | 2.25                     | 0.51              |
| 1:A1:381:ARG:HA   | 1:A1:384:LEU:HD12  | 1.91                     | 0.51              |
| 4:D1:26:ILE:HG21  | 4:D1:54:VAL:HG22   | 1.92                     | 0.51              |
| 4:D1:32:VAL:HG11  | 4:D1:186:VAL:CG2   | 2.41                     | 0.51              |
| 10:J1:49:GLY:HA2  | 10:J1:54:HIS:HB3   | 1.92                     | 0.51              |
| 10:J1:51:LEU:H    | 10:J1:54:HIS:HD2   | 1.57                     | 0.51              |
| 1:M1:213:GLN:CB   | 1:M1:215:HIS:NE2   | 2.70                     | 0.51              |
| 2:N1:258:VAL:CG1  | 2:N1:321:LEU:HD22  | 2.40                     | 0.51              |
| 3:O1:117:VAL:N    | 69:O1:402:HEM:HBC2 | 2.25                     | 0.51              |
| 5:Q1:119:ASP:HB3  | 5:Q1:179:ASN:ND2   | 2.26                     | 0.51              |
| 5:Q1:119:ASP:OD1  | 5:Q1:120:PRO:HD2   | 2.09                     | 0.51              |
| 19:A2:238:PHE:CE2 | 23:E2:138:GLY:O    | 2.63                     | 0.51              |
| 20:B2:97:LEU:HB3  | 20:B2:111:PRO:CB   | 2.40                     | 0.51              |
| 30:L2:76:PRO:HD2  | 34:Q2:127:LYS:HG2  | 1.91                     | 0.51              |
| 2:B1:178:CYS:SG   | 2:B1:179:PRO:HD2   | 2.51                     | 0.51              |
| 3:C1:153:ILE:HD12 | 3:C1:153:ILE:N     | 2.25                     | 0.51              |
| 6:F1:7:SER:O      | 6:F1:11:ARG:HD2    | 2.10                     | 0.51              |
| 1:M1:134:ILE:HD13 | 1:M1:137:GLU:HG3   | 1.91                     | 0.51              |
| 4:P1:27:ARG:NH1   | 10:V1:58:LYS:CE    | 2.72                     | 0.51              |
| 4:P1:82:MET:HE2   | 4:P1:86:LYS:NZ     | 2.25                     | 0.51              |
| 4:P1:138:PRO:HB3  | 8:T1:55:THR:CA     | 2.40                     | 0.51              |
| 4:P1:213:GLY:O    | 4:P1:217:PRO:HG3   | 2.11                     | 0.51              |
| 16:72:165:VAL:O   | 16:72:169:MET:N    | 2.42                     | 0.51              |
| 19:A2:587:ALA:HB1 | 19:A2:591:GLU:HB2  | 1.91                     | 0.51              |
| 35:R2:281:PHE:HB3 | 35:R2:286:ARG:HD3  | 1.91                     | 0.51              |
| 35:R2:329:LEU:HG  | 35:R2:331:HIS:H    | 1.76                     | 0.51              |
| 51:j2:108:THR:HA  | 54:g2:78:GLN:HA    | 1.92                     | 0.51              |
| 1:A1:279:HIS:CE1  | 1:A1:284:TYR:OH    | 2.63                     | 0.51              |
| 2:B1:34:VAL:HG11  | 2:B1:386:ALA:CB    | 2.41                     | 0.51              |
| 2:B1:412:ASN:O    | 2:B1:415:LYS:HB2   | 2.11                     | 0.51              |
| 1:M1:46:ARG:NH1   | 1:M1:316:ASP:OD1   | 2.40                     | 0.51              |
| 1:M1:158:PHE:HE1  | 1:M1:317:THR:HG21  | 1.72                     | 0.51              |
| 1:M1:428:ILE:CG2  | 1:M1:431:LEU:CD2   | 2.85                     | 0.51              |
| 2:N1:102:ARG:HH12 | 2:N1:175:SER:HA    | 1.75                     | 0.51              |
| 2:N1:141:GLN:OE1  | 2:N1:183:ILE:O     | 2.29                     | 0.51              |
| 3:O1:19:ILE:HG23  | 3:O1:221:HIS:HB2   | 1.92                     | 0.51              |
| 3:O1:85:ASN:O     | 3:O1:86:GLY:C      | 2.53                     | 0.51              |
| 3:O1:166:GLY:HA3  | 3:O1:177:ARG:NH2   | 2.26                     | 0.51              |
| 4:P1:48:TYR:CD2   | 4:P1:65:ALA:HB2    | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:D2:75:ASN:OD1   | 22:D2:78:ARG:NH2   | 2.43                     | 0.51              |
| 56:A3:240:HIS:HB3  | 56:A3:241:PRO:HD3  | 1.92                     | 0.51              |
| 62:G3:42:ARG:HH11  | 62:G3:42:ARG:HG3   | 1.74                     | 0.51              |
| 1:A1:41:ILE:HD12   | 1:A1:41:ILE:N      | 2.24                     | 0.51              |
| 1:A1:53:ASN:HB3    | 1:A1:170:PRO:HD2   | 1.91                     | 0.51              |
| 1:A1:200:ALA:HB2   | 1:A1:375:VAL:HG12  | 1.92                     | 0.51              |
| 2:B1:162:ASN:HB3   | 2:B1:244:ILE:CG2   | 2.40                     | 0.51              |
| 2:B1:429:ASN:C     | 2:B1:429:ASN:HD22  | 2.19                     | 0.51              |
| 3:C1:125:ALA:O     | 3:C1:126:THR:C     | 2.53                     | 0.51              |
| 3:C1:344:GLU:O     | 3:C1:348:ILE:HG13  | 2.11                     | 0.51              |
| 2:N1:67:HIS:CE1    | 2:N1:177:TYR:HD1   | 2.28                     | 0.51              |
| 2:N1:262:ALA:CB    | 2:N1:268:GLU:HB3   | 2.41                     | 0.51              |
| 2:N1:435:PHE:H     | 2:N1:438:GLU:HB2   | 1.74                     | 0.51              |
| 3:O1:153:ILE:HD12  | 3:O1:153:ILE:H     | 1.74                     | 0.51              |
| 4:P1:43:MET:HA     | 4:P1:112:ASP:OD1   | 2.10                     | 0.51              |
| 14:42:301:ILE:O    | 14:42:304:GLN:NE2  | 2.43                     | 0.51              |
| 19:A2:199:GLY:HA3  | 19:A2:204:MET:HA   | 1.93                     | 0.51              |
| 19:A2:380:ASP:OD1  | 19:A2:380:ASP:N    | 2.38                     | 0.51              |
| 19:A2:557:ARG:HG3  | 19:A2:560:LEU:HD23 | 1.91                     | 0.51              |
| 36:S2:182:THR:HG23 | 36:S2:183:ILE:HG13 | 1.92                     | 0.51              |
| 1:A1:39:VAL:CG1    | 1:A1:41:ILE:HD11   | 2.35                     | 0.51              |
| 1:A1:106:LEU:HB3   | 1:A1:107:PRO:CD    | 2.41                     | 0.51              |
| 1:A1:211:LEU:O     | 1:A1:211:LEU:HD12  | 2.11                     | 0.51              |
| 2:B1:148:LYS:HD2   | 2:B1:178:CYS:O     | 2.10                     | 0.51              |
| 2:B1:261:SER:HB3   | 2:B1:321:LEU:N     | 2.25                     | 0.51              |
| 3:C1:184:ILE:O     | 3:C1:188:ILE:HD12  | 2.10                     | 0.51              |
| 3:C1:331:ASP:OD1   | 3:C1:354:ALA:HB1   | 2.11                     | 0.51              |
| 4:D1:2:ASP:HB3     | 4:D1:156:GLN:NE2   | 2.26                     | 0.51              |
| 1:M1:106:LEU:HB3   | 1:M1:107:PRO:CD    | 2.40                     | 0.51              |
| 2:N1:303:VAL:CG1   | 2:N1:304:HIS:H     | 2.24                     | 0.51              |
| 5:Q1:86:ASN:HD21   | 5:Q1:97:PHE:HD2    | 1.54                     | 0.51              |
| 14:42:276:CYS:SG   | 14:42:406:TYR:OH   | 2.65                     | 0.51              |
| 52:12:46:LEU:HG    | 52:12:49:ILE:HD11  | 1.91                     | 0.51              |
| 52:12:210:GLY:HA2  | 52:12:213:VAL:HG12 | 1.91                     | 0.51              |
| 57:B3:136:LEU:HB3  | 57:B3:193:TYR:CD2  | 2.46                     | 0.51              |
| 1:A1:84:ALA:HB2    | 1:A1:101:ALA:CB    | 2.37                     | 0.51              |
| 1:A1:329:MET:HA    | 1:A1:430:GLN:OE1   | 2.10                     | 0.51              |
| 2:B1:275:LEU:HD11  | 2:B1:279:LEU:CD1   | 2.41                     | 0.51              |
| 2:B1:305:GLN:CB    | 2:B1:306:PRO:HD3   | 2.31                     | 0.51              |
| 2:B1:375:SER:OG    | 2:B1:376:GLU:N     | 2.42                     | 0.51              |
| 3:C1:177:ARG:O     | 3:C1:181:PHE:HD2   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:240:MET:SD    | 3:C1:243:VAL:HG11  | 2.51                     | 0.51              |
| 3:C1:277:ALA:O     | 3:C1:278:TYR:C     | 2.52                     | 0.51              |
| 3:C1:282:ARG:O     | 3:C1:284:ILE:N     | 2.43                     | 0.51              |
| 4:D1:27:ARG:NH1    | 10:J1:58:LYS:HE3   | 2.26                     | 0.51              |
| 6:F1:104:ARG:O     | 6:F1:105:GLU:C     | 2.53                     | 0.51              |
| 7:G1:33:GLY:O      | 7:G1:37:VAL:HB     | 2.11                     | 0.51              |
| 8:H1:27:LEU:O      | 8:H1:30:CYS:N      | 2.38                     | 0.51              |
| 8:H1:70:ALA:HA     | 8:H1:73:LEU:HD22   | 1.92                     | 0.51              |
| 1:M1:131:ARG:O     | 1:M1:132:ASP:C     | 2.53                     | 0.51              |
| 1:M1:446:PHE:HE2   | 3:O1:6:LYS:HZ1     | 1.58                     | 0.51              |
| 2:N1:129:ALA:H     | 2:N1:130:PRO:HD3   | 1.76                     | 0.51              |
| 2:N1:393:THR:HG22  | 2:N1:394:PRO:O     | 2.10                     | 0.51              |
| 3:O1:196:HIS:CE1   | 69:O1:402:HEM:ND   | 2.78                     | 0.51              |
| 3:O1:357:LEU:O     | 3:O1:361:LEU:HG    | 2.10                     | 0.51              |
| 6:R1:37:ILE:HG23   | 6:R1:37:ILE:O      | 2.11                     | 0.51              |
| 6:R1:49:ARG:NH2    | 6:R1:100:GLU:OE2   | 2.37                     | 0.51              |
| 19:A2:403:VAL:HG12 | 19:A2:432:ILE:HB   | 1.92                     | 0.51              |
| 20:B2:140:ASP:OD2  | 20:B2:143:SER:OG   | 2.28                     | 0.51              |
| 26:H2:21:GLN:O     | 26:H2:25:GLN:NE2   | 2.43                     | 0.51              |
| 35:R2:171:ASN:HD21 | 35:R2:324:THR:HB   | 1.76                     | 0.51              |
| 57:B3:1:MET:SD     | 57:B3:133:LEU:CD1  | 2.98                     | 0.51              |
| 2:B1:85:ILE:O      | 2:B1:89:ILE:HG13   | 2.10                     | 0.51              |
| 2:B1:350:GLY:HA2   | 2:B1:411:ILE:HG21  | 1.92                     | 0.51              |
| 3:C1:107:TYR:OH    | 3:C1:308:HIS:ND1   | 2.09                     | 0.51              |
| 5:E1:15:ARG:HH21   | 5:E1:32:ARG:CB     | 2.24                     | 0.51              |
| 1:M1:162:PRO:O     | 1:M1:165:GLN:NE2   | 2.42                     | 0.51              |
| 1:M1:389:ARG:C     | 1:M1:391:PRO:HD3   | 2.36                     | 0.51              |
| 2:N1:209:LEU:HG    | 2:N1:209:LEU:O     | 2.09                     | 0.51              |
| 2:N1:261:SER:HB3   | 2:N1:321:LEU:N     | 2.26                     | 0.51              |
| 3:O1:91:PHE:O      | 3:O1:92:ILE:C      | 2.52                     | 0.51              |
| 4:P1:220:TYR:O     | 4:P1:221:ALA:C     | 2.53                     | 0.51              |
| 5:Q1:135:LEU:HD22  | 5:Q1:182:VAL:HG22  | 1.92                     | 0.51              |
| 5:Q1:191:ASP:OD1   | 5:Q1:191:ASP:N     | 2.42                     | 0.51              |
| 29:K2:65:LEU:HB3   | 29:K2:77:VAL:HG23  | 1.92                     | 0.51              |
| 39:V2:48:TRP:O     | 39:V2:52:LYS:NZ    | 2.39                     | 0.51              |
| 56:A3:250:GLY:O    | 56:A3:254:ILE:HG12 | 2.11                     | 0.51              |
| 56:A3:347:LEU:HG   | 56:A3:383:MET:HE3  | 1.93                     | 0.51              |
| 1:A1:426:GLY:H     | 1:A1:428:ILE:HG12  | 1.66                     | 0.51              |
| 2:B1:88:GLY:O      | 2:B1:91:ALA:HB3    | 2.11                     | 0.51              |
| 2:B1:112:LEU:O     | 2:B1:113:ARG:C     | 2.54                     | 0.51              |
| 2:B1:200:THR:OG1   | 2:B1:201:SER:N     | 2.44                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B1:383:GLY:O    | 2:B1:386:ALA:HB3   | 2.10                     | 0.51              |
| 3:C1:105:GLY:HA2  | 3:C1:107:TYR:CD1   | 2.46                     | 0.51              |
| 4:D1:42:SER:O     | 4:D1:112:ASP:OD1   | 2.29                     | 0.51              |
| 4:D1:102:ARG:HG2  | 4:D1:109:LEU:HB2   | 1.93                     | 0.51              |
| 1:M1:51:LYS:C     | 1:M1:53:ASN:H      | 2.19                     | 0.51              |
| 1:M1:55:ALA:O     | 1:M1:58:PHE:N      | 2.39                     | 0.51              |
| 1:M1:82:MET:SD    | 1:M1:105:ASP:HB3   | 2.51                     | 0.51              |
| 1:M1:124:ASP:O    | 1:M1:128:GLU:HG2   | 2.11                     | 0.51              |
| 1:M1:279:HIS:ND1  | 1:M1:284:TYR:OH    | 2.39                     | 0.51              |
| 1:M1:329:MET:HA   | 1:M1:430:GLN:OE1   | 2.11                     | 0.51              |
| 1:M1:408:ARG:O    | 1:M1:412:SER:OG    | 2.28                     | 0.51              |
| 3:O1:30:TRP:HA    | 3:O1:33:PHE:HE2    | 1.75                     | 0.51              |
| 4:P1:79:GLU:O     | 4:P1:80:MET:C      | 2.52                     | 0.51              |
| 4:P1:79:GLU:HB3   | 4:P1:82:MET:HB2    | 1.93                     | 0.51              |
| 4:P1:224:ARG:NH2  | 7:S1:27:PRO:HD2    | 2.26                     | 0.51              |
| 35:R2:168:SER:OG  | 35:R2:169:HIS:N    | 2.44                     | 0.51              |
| 35:R2:326:ASP:O   | 35:R2:328:ILE:HG13 | 2.10                     | 0.51              |
| 2:B1:115:ASP:HA   | 2:B1:118:ILE:HD12  | 1.92                     | 0.51              |
| 4:D1:164:ILE:HG21 | 4:D1:182:VAL:HG12  | 1.92                     | 0.51              |
| 2:N1:308:ASP:OD2  | 9:U1:54:SER:O      | 2.29                     | 0.51              |
| 9:U1:58:GLN:HB3   | 9:U1:78:TYR:HB2    | 1.92                     | 0.51              |
| 12:22:63:GLN:HE21 | 12:22:114:TRP:HZ2  | 1.59                     | 0.51              |
| 59:D3:40:LEU:HD22 | 59:D3:59:LEU:HD13  | 1.92                     | 0.51              |
| 1:A1:279:HIS:CE1  | 1:A1:284:TYR:HH    | 2.29                     | 0.50              |
| 1:A1:378:ASP:O    | 1:A1:382:SER:HB2   | 2.11                     | 0.50              |
| 2:B1:77:THR:HG22  | 2:B1:130:PRO:N     | 2.24                     | 0.50              |
| 2:B1:304:HIS:CG   | 2:B1:305:GLN:H     | 2.29                     | 0.50              |
| 3:C1:100:ARG:NH2  | 69:C1:402:HEM:O2A  | 2.44                     | 0.50              |
| 3:C1:135:TRP:CH2  | 3:C1:170:VAL:HG12  | 2.41                     | 0.50              |
| 3:C1:312:GLN:O    | 3:C1:313:ARG:C     | 2.53                     | 0.50              |
| 3:C1:312:GLN:NE2  | 3:C1:317:PHE:HB2   | 2.25                     | 0.50              |
| 3:C1:341:GLN:O    | 3:C1:342:PRO:C     | 2.52                     | 0.50              |
| 3:C1:373:GLU:HB3  | 6:F1:20:TYR:OH     | 2.12                     | 0.50              |
| 4:D1:120:ARG:HH11 | 4:D1:120:ARG:CG    | 2.24                     | 0.50              |
| 6:F1:96:GLU:O     | 6:F1:99:ARG:N      | 2.44                     | 0.50              |
| 7:G1:80:ASP:O     | 7:G1:81:ARG:HB2    | 2.10                     | 0.50              |
| 1:M1:392:LEU:O    | 1:M1:392:LEU:HG    | 2.09                     | 0.50              |
| 2:N1:47:ILE:CG2   | 2:N1:48:GLY:N      | 2.72                     | 0.50              |
| 3:O1:130:GLY:O    | 69:O1:401:HEM:HAA1 | 2.11                     | 0.50              |
| 3:O1:147:THR:HG21 | 3:O1:165:TRP:CD1   | 2.46                     | 0.50              |
| 4:P1:14:HIS:HA    | 4:P1:19:SER:HB3    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:P1:24:THR:O      | 4:P1:25:SER:C      | 2.54                     | 0.50              |
| 5:Q1:45:VAL:HG22   | 10:V1:28:ALA:N     | 2.26                     | 0.50              |
| 5:Q1:51:ALA:O      | 5:Q1:55:VAL:HG23   | 2.11                     | 0.50              |
| 9:U1:58:GLN:O      | 9:U1:59:ALA:HB2    | 2.11                     | 0.50              |
| 9:U1:78:TYR:OXT    | 9:U1:78:TYR:CD1    | 2.64                     | 0.50              |
| 18:92:54:ASP:OD1   | 18:92:60:TYR:OH    | 2.29                     | 0.50              |
| 19:A2:126:LEU:HD11 | 20:B2:373:THR:O    | 2.11                     | 0.50              |
| 31:N2:62:GLU:OE2   | 31:N2:71:ARG:NH1   | 2.37                     | 0.50              |
| 34:Q2:111:VAL:HG12 | 34:Q2:117:TRP:HB2  | 1.93                     | 0.50              |
| 47:d2:18:ASP:O     | 47:d2:20:LEU:N     | 2.43                     | 0.50              |
| 56:A3:75:ILE:O     | 56:A3:79:GLY:HA3   | 2.11                     | 0.50              |
| 56:A3:377:PHE:HA   | 56:A3:380:VAL:HG22 | 1.93                     | 0.50              |
| 1:A1:26:ALA:O      | 1:A1:27:SER:HB3    | 2.10                     | 0.50              |
| 1:A1:236:PHE:HB2   | 5:E1:25:SER:HB2    | 1.93                     | 0.50              |
| 1:A1:291:SER:HB3   | 2:B1:87:ARG:HD3    | 1.93                     | 0.50              |
| 2:B1:166:ALA:HB2   | 2:B1:244:ILE:CD1   | 2.41                     | 0.50              |
| 6:F1:23:ALA:O      | 6:F1:24:ALA:C      | 2.52                     | 0.50              |
| 1:M1:143:THR:HG21  | 9:U1:48:SER:N      | 2.08                     | 0.50              |
| 1:M1:256:ALA:CA    | 1:M1:320:LEU:O     | 2.59                     | 0.50              |
| 3:O1:152:ALA:N     | 3:O1:287:LYS:NZ    | 2.59                     | 0.50              |
| 5:Q1:51:ALA:O      | 5:Q1:52:LYS:C      | 2.54                     | 0.50              |
| 11:W1:18:VAL:CB    | 11:W1:19:PRO:HD3   | 2.41                     | 0.50              |
| 20:B2:203:MET:HE1  | 20:B2:254:ARG:HB3  | 1.93                     | 0.50              |
| 23:E2:189:LYS:HB2  | 38:U2:124:TYR:CZ   | 2.47                     | 0.50              |
| 53:62:172:ILE:HA   | 53:62:175:ASN:HD22 | 1.76                     | 0.50              |
| 1:A1:279:HIS:ND1   | 1:A1:284:TYR:OH    | 2.42                     | 0.50              |
| 1:A1:331:ILE:CD1   | 1:A1:427:PRO:O     | 2.58                     | 0.50              |
| 2:B1:352:LEU:HD23  | 2:B1:411:ILE:HD11  | 1.92                     | 0.50              |
| 4:D1:230:LEU:O     | 4:D1:233:ARG:HB2   | 2.12                     | 0.50              |
| 7:G1:52:PHE:O      | 7:G1:53:VAL:C      | 2.54                     | 0.50              |
| 1:M1:294:LEU:CD2   | 1:M1:337:VAL:HG12  | 2.41                     | 0.50              |
| 1:M1:426:GLY:HA2   | 1:M1:427:PRO:C     | 2.36                     | 0.50              |
| 2:N1:304:HIS:CD2   | 2:N1:305:GLN:H     | 2.30                     | 0.50              |
| 3:O1:152:ALA:HB2   | 3:O1:287:LYS:NZ    | 2.26                     | 0.50              |
| 3:O1:160:LEU:O     | 3:O1:164:ILE:HD12  | 2.11                     | 0.50              |
| 5:Q1:114:VAL:CG1   | 5:Q1:115:SER:N     | 2.73                     | 0.50              |
| 10:V1:52:TRP:O     | 10:V1:53:LYS:C     | 2.53                     | 0.50              |
| 12:22:300:THR:HG23 | 12:22:301:THR:HG23 | 1.93                     | 0.50              |
| 19:A2:129:PRO:CB   | 27:I2:114:TYR:HE1  | 2.24                     | 0.50              |
| 52:12:131:GLY:HA2  | 52:12:134:ARG:HE   | 1.76                     | 0.50              |
| 56:A3:40:GLU:HG2   | 56:A3:54:TYR:CD1   | 2.47                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:C3:119:THR:O   | 62:G3:52:HIS:CE1   | 2.63                     | 0.50              |
| 1:A1:64:PHE:HE2   | 1:A1:88:ALA:HB2    | 1.75                     | 0.50              |
| 1:A1:106:LEU:HD22 | 1:A1:203:LEU:HD13  | 1.93                     | 0.50              |
| 1:A1:296:SER:O    | 1:A1:297:ILE:C     | 2.55                     | 0.50              |
| 2:B1:38:LEU:O     | 2:B1:40:ASN:N      | 2.45                     | 0.50              |
| 3:C1:46:LEU:O     | 3:C1:50:PHE:HD1    | 1.94                     | 0.50              |
| 3:C1:132:VAL:HA   | 3:C1:139:SER:CB    | 2.42                     | 0.50              |
| 3:C1:164:ILE:O    | 3:C1:177:ARG:NH1   | 2.42                     | 0.50              |
| 3:C1:276:PHE:HE2  | 3:C1:297:SER:OG    | 1.95                     | 0.50              |
| 4:D1:46:VAL:HG12  | 4:D1:47:ALA:O      | 2.10                     | 0.50              |
| 4:D1:138:PRO:CB   | 8:H1:55:THR:CA     | 2.90                     | 0.50              |
| 4:D1:161:ALA:O    | 4:D1:163:PRO:N     | 2.45                     | 0.50              |
| 7:G1:54:ALA:O     | 7:G1:58:VAL:HG23   | 2.12                     | 0.50              |
| 3:O1:191:ALA:O    | 3:O1:195:VAL:HG23  | 2.12                     | 0.50              |
| 4:P1:69:GLU:HA    | 4:P1:73:GLY:HA2    | 1.93                     | 0.50              |
| 4:P1:72:ASP:OD1   | 4:P1:76:GLU:OE1    | 2.29                     | 0.50              |
| 5:Q1:18:VAL:HG11  | 5:Q1:32:ARG:NH1    | 2.27                     | 0.50              |
| 10:V1:21:ALA:O    | 10:V1:22:LEU:C     | 2.53                     | 0.50              |
| 48:f2:70:GLU:H    | 48:f2:73:HIS:HB3   | 1.75                     | 0.50              |
| 1:A1:64:PHE:HA    | 1:A1:75:LEU:CD2    | 2.42                     | 0.50              |
| 1:A1:142:ASP:OD2  | 5:E1:1:SER:HB3     | 2.11                     | 0.50              |
| 3:C1:246:ALA:HB1  | 3:C1:249:LEU:HB2   | 1.94                     | 0.50              |
| 3:C1:280:ILE:HD13 | 3:C1:280:ILE:N     | 2.27                     | 0.50              |
| 2:N1:47:ILE:HG22  | 2:N1:48:GLY:H      | 1.76                     | 0.50              |
| 2:N1:76:THR:HG21  | 2:N1:133:ARG:CZ    | 2.42                     | 0.50              |
| 2:N1:97:SER:HA    | 9:U1:70:LEU:HB2    | 1.94                     | 0.50              |
| 3:O1:10:LEU:HD12  | 3:O1:13:ILE:HD11   | 1.92                     | 0.50              |
| 3:O1:115:ILE:HD13 | 3:O1:115:ILE:N     | 2.26                     | 0.50              |
| 3:O1:242:LEU:HD21 | 3:O1:250:LEU:CD2   | 2.41                     | 0.50              |
| 4:P1:10:TYR:HD1   | 8:T1:74:PHE:CE1    | 2.29                     | 0.50              |
| 4:P1:23:HIS:CD2   | 10:V1:50:LYS:O     | 2.65                     | 0.50              |
| 10:V1:32:GLU:CG   | 10:V1:33:ARG:N     | 2.74                     | 0.50              |
| 19:A2:423:LEU:CD1 | 25:G2:169:ARG:O    | 2.60                     | 0.50              |
| 19:A2:613:PRO:CB  | 38:U2:134:ILE:HD13 | 2.38                     | 0.50              |
| 21:C2:167:TRP:CD1 | 21:C2:170:ARG:HH12 | 2.30                     | 0.50              |
| 33:P2:41:LEU:HD12 | 33:P2:42:PRO:HD2   | 1.94                     | 0.50              |
| 58:C3:18:LEU:HD22 | 58:C3:22:LEU:HD22  | 1.92                     | 0.50              |
| 2:B1:197:ASN:HB2  | 2:B1:198:HIS:CD2   | 2.46                     | 0.50              |
| 3:C1:147:THR:O    | 3:C1:150:LEU:HB2   | 2.11                     | 0.50              |
| 3:C1:163:TRP:CE2  | 5:Q1:62:MET:HE2    | 2.46                     | 0.50              |
| 4:D1:30:PHE:CE1   | 4:D1:50:HIS:CE1    | 2.99                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D1:138:PRO:HB3   | 8:H1:55:THR:HA     | 1.94                     | 0.50              |
| 5:E1:71:MET:O      | 5:E1:72:SER:C      | 2.54                     | 0.50              |
| 1:M1:53:ASN:CG     | 1:M1:165:GLN:HB2   | 2.35                     | 0.50              |
| 2:N1:109:VAL:HG22  | 2:N1:119:LEU:CD2   | 2.41                     | 0.50              |
| 2:N1:198:HIS:HE1   | 2:N1:233:SER:CB    | 2.23                     | 0.50              |
| 2:N1:340:ALA:O     | 2:N1:344:VAL:HG23  | 2.12                     | 0.50              |
| 2:N1:350:GLY:HA2   | 2:N1:411:ILE:HG21  | 1.93                     | 0.50              |
| 4:P1:146:GLY:O     | 4:P1:148:TYR:CD1   | 2.65                     | 0.50              |
| 6:R1:58:ARG:HG2    | 6:R1:58:ARG:NH1    | 2.25                     | 0.50              |
| 18:92:111:ARG:HH12 | 19:A2:193:ASP:HA   | 1.77                     | 0.50              |
| 20:B2:272:THR:HA   | 20:B2:275:ILE:HD12 | 1.93                     | 0.50              |
| 42:Y2:46:ARG:HA    | 42:Y2:49:GLN:HE22  | 1.76                     | 0.50              |
| 54:g2:141:ASP:OD1  | 54:g2:141:ASP:N    | 2.44                     | 0.50              |
| 55:e2:70:THR:C     | 55:e2:72:TYR:N     | 2.61                     | 0.50              |
| 56:A3:168:ILE:HG21 | 56:A3:189:MET:HG3  | 1.94                     | 0.50              |
| 56:A3:232:GLN:HB2  | 56:A3:292:MET:HE3  | 1.93                     | 0.50              |
| 61:F3:37:LYS:HD3   | 61:F3:37:LYS:N     | 2.27                     | 0.50              |
| 63:H3:60:TYR:C     | 63:H3:60:TYR:CD1   | 2.88                     | 0.50              |
| 1:A1:48:GLU:HB3    | 1:A1:52:ASN:O      | 2.10                     | 0.50              |
| 2:B1:429:ASN:ND2   | 2:N1:60:SER:OG     | 2.45                     | 0.50              |
| 4:D1:72:ASP:OD1    | 4:D1:76:GLU:OE1    | 2.30                     | 0.50              |
| 9:I1:62:ARG:H      | 9:I1:63:PRO:HD2    | 1.76                     | 0.50              |
| 10:J1:49:GLY:HA2   | 10:J1:54:HIS:HB2   | 1.91                     | 0.50              |
| 1:M1:30:SER:N      | 1:M1:201:GLY:O     | 2.44                     | 0.50              |
| 4:P1:7:PRO:HB2     | 4:P1:125:ASP:HB3   | 1.93                     | 0.50              |
| 14:42:214:LEU:HD11 | 53:62:558:LEU:HB3  | 1.92                     | 0.50              |
| 19:A2:238:PHE:CB   | 23:E2:140:ARG:HB3  | 2.40                     | 0.50              |
| 35:R2:281:PHE:HD1  | 35:R2:286:ARG:HA   | 1.75                     | 0.50              |
| 53:62:103:PHE:O    | 53:62:107:TYR:N    | 2.40                     | 0.50              |
| 57:B3:139:ASP:OD1  | 57:B3:140:ASN:N    | 2.44                     | 0.50              |
| 1:A1:124:ASP:O     | 1:A1:128:GLU:HG2   | 2.11                     | 0.50              |
| 1:A1:252:HIS:CD2   | 1:A1:325:VAL:HG22  | 2.47                     | 0.50              |
| 1:A1:272:VAL:O     | 1:A1:275:ALA:HB3   | 2.12                     | 0.50              |
| 2:B1:170:ASN:CG    | 2:B1:171:ALA:N     | 2.70                     | 0.50              |
| 2:B1:275:LEU:HD12  | 2:B1:275:LEU:O     | 2.12                     | 0.50              |
| 3:C1:4:ILE:O       | 3:C1:5:ARG:C       | 2.53                     | 0.50              |
| 6:F1:51:PRO:CD     | 2:N1:134:ARG:HH12  | 2.24                     | 0.50              |
| 1:M1:120:CYS:O     | 1:M1:122:LEU:HG    | 2.12                     | 0.50              |
| 2:N1:130:PRO:HB2   | 2:N1:132:PHE:CE1   | 2.46                     | 0.50              |
| 2:N1:196:GLN:HG2   | 2:N1:197:ASN:OD1   | 2.12                     | 0.50              |
| 2:N1:257:LEU:CD1   | 2:N1:424:MET:HB2   | 2.40                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N1:279:LEU:CD2   | 2:N1:344:VAL:HG22  | 2.40                     | 0.50              |
| 4:P1:30:PHE:HD1    | 4:P1:189:PHE:CE1   | 2.29                     | 0.50              |
| 4:P1:138:PRO:CB    | 8:T1:55:THR:CA     | 2.90                     | 0.50              |
| 5:Q1:152:ASP:N     | 5:Q1:164:HIS:ND1   | 2.59                     | 0.50              |
| 7:S1:64:GLN:O      | 7:S1:65:GLU:C      | 2.55                     | 0.50              |
| 20:B2:144:MET:HE3  | 20:B2:222:MET:HB3  | 1.93                     | 0.50              |
| 39:V2:55:ARG:NH2   | 52:12:312:SER:OG   | 2.32                     | 0.50              |
| 1:A1:113:LEU:HA    | 1:A1:116:ILE:HD12  | 1.92                     | 0.50              |
| 2:B1:45:SER:HB2    | 2:B1:210:GLY:HA3   | 1.93                     | 0.50              |
| 2:B1:372:VAL:O     | 2:B1:372:VAL:HG12  | 2.11                     | 0.50              |
| 3:C1:26:ASN:ND2    | 3:C1:208:PRO:HD2   | 2.27                     | 0.50              |
| 3:C1:106:SER:CB    | 69:C1:402:HEM:HBD2 | 2.41                     | 0.50              |
| 4:D1:33:TYR:O      | 4:D1:37:CYS:HB2    | 2.12                     | 0.50              |
| 4:D1:82:MET:SD     | 4:D1:86:LYS:NZ     | 2.82                     | 0.50              |
| 9:I1:62:ARG:N      | 9:I1:63:PRO:CD     | 2.75                     | 0.50              |
| 2:N1:237:ALA:HB2   | 2:N1:318:ASP:CG    | 2.37                     | 0.50              |
| 3:O1:378:LYS:O     | 3:O1:378:LYS:HD3   | 2.11                     | 0.50              |
| 4:P1:117:VAL:CG1   | 4:P1:191:ARG:HH11  | 2.25                     | 0.50              |
| 4:P1:134:TYR:HE2   | 4:P1:163:PRO:CG    | 2.25                     | 0.50              |
| 4:P1:165:TYR:H     | 4:P1:168:VAL:CG2   | 2.24                     | 0.50              |
| 5:Q1:34:GLY:CA     | 10:V1:10:TYR:HD1   | 2.22                     | 0.50              |
| 12:22:245:LEU:HD22 | 12:22:301:THR:HG21 | 1.94                     | 0.50              |
| 17:82:321:GLY:N    | 17:82:351:THR:OG1  | 2.43                     | 0.50              |
| 20:B2:326:CYS:HA   | 20:B2:329:ARG:HG2  | 1.94                     | 0.50              |
| 35:R2:84:HIS:CD2   | 35:R2:87:GLU:H     | 2.30                     | 0.50              |
| 1:A1:22:GLY:O      | 1:A1:24:ARG:HG2    | 2.12                     | 0.49              |
| 1:A1:63:ALA:HB2    | 1:A1:97:TYR:HE2    | 1.76                     | 0.49              |
| 1:A1:335:MET:CE    | 1:A1:339:GLN:HG3   | 2.42                     | 0.49              |
| 1:A1:395:TRP:O     | 1:A1:398:ARG:N     | 2.45                     | 0.49              |
| 7:G1:40:ARG:O      | 7:G1:41:THR:C      | 2.55                     | 0.49              |
| 1:M1:40:TRP:HZ2    | 1:M1:377:GLU:HB2   | 1.75                     | 0.49              |
| 1:M1:92:ARG:HD2    | 1:M1:163:LEU:CD1   | 2.37                     | 0.49              |
| 2:N1:185:LYS:HG3   | 2:N1:185:LYS:O     | 2.11                     | 0.49              |
| 2:N1:206:LEU:CD1   | 2:N1:224:LEU:HD11  | 2.41                     | 0.49              |
| 3:O1:164:ILE:O     | 3:O1:177:ARG:NH1   | 2.44                     | 0.49              |
| 3:O1:317:PHE:CD1   | 6:R1:26:PHE:HB3    | 2.47                     | 0.49              |
| 4:P1:35:GLN:HB2    | 4:P1:169:LEU:CD1   | 2.42                     | 0.49              |
| 4:P1:138:PRO:HB3   | 8:T1:54:CYS:C      | 2.38                     | 0.49              |
| 4:P1:232:SER:CB    | 7:S1:23:GLN:OE1    | 2.59                     | 0.49              |
| 5:Q1:9:ASP:OD1     | 5:Q1:11:SER:OG     | 2.30                     | 0.49              |
| 5:Q1:119:ASP:HB3   | 5:Q1:179:ASN:HD21  | 1.76                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:U1:62:ARG:N      | 9:U1:63:PRO:CD     | 2.75                     | 0.49              |
| 17:82:119:GLU:O    | 17:82:159:ARG:NH2  | 2.45                     | 0.49              |
| 18:92:227:PRO:HD2  | 18:92:231:LEU:HA   | 1.93                     | 0.49              |
| 21:C2:188:ARG:NH1  | 21:C2:193:TYR:O    | 2.45                     | 0.49              |
| 23:E2:188:GLU:OE1  | 38:U2:127:TYR:OH   | 2.30                     | 0.49              |
| 59:D3:64:PHE:CE1   | 60:E3:66:ARG:HD2   | 2.47                     | 0.49              |
| 1:A1:158:PHE:O     | 1:A1:164:ALA:HB2   | 2.12                     | 0.49              |
| 1:A1:408:ARG:HH12  | 11:K1:15:ARG:CD    | 2.25                     | 0.49              |
| 2:B1:381:GLU:O     | 2:B1:384:SER:OG    | 2.24                     | 0.49              |
| 3:C1:37:LEU:HD21   | 3:C1:94:LEU:HD13   | 1.93                     | 0.49              |
| 3:C1:43:LEU:O      | 3:C1:44:GLN:C      | 2.51                     | 0.49              |
| 3:C1:278:TYR:O     | 3:C1:279:ALA:C     | 2.55                     | 0.49              |
| 4:D1:138:PRO:O     | 4:D1:141:VAL:HB    | 2.12                     | 0.49              |
| 1:M1:3:THR:O       | 1:M1:4:TYR:C       | 2.54                     | 0.49              |
| 3:O1:122:THR:HB    | 3:O1:189:ILE:HD13  | 1.95                     | 0.49              |
| 10:V1:60:GLU:O     | 10:V1:60:GLU:HG3   | 2.11                     | 0.49              |
| 49:h2:120:ARG:HH22 | 54:g2:65:HIS:HA    | 1.77                     | 0.49              |
| 57:B3:186:SER:HB3  | 57:B3:213:LEU:CD2  | 2.42                     | 0.49              |
| 1:A1:171:SER:O     | 1:A1:174:VAL:HB    | 2.13                     | 0.49              |
| 1:A1:349:ALA:HB3   | 1:A1:408:ARG:HG2   | 1.95                     | 0.49              |
| 2:B1:255:ALA:HA    | 2:B1:425:ALA:O     | 2.12                     | 0.49              |
| 3:C1:338:ILE:HA    | 3:C1:341:GLN:CG    | 2.43                     | 0.49              |
| 1:M1:307:PHE:HA    | 1:M1:323:HIS:O     | 2.12                     | 0.49              |
| 3:O1:344:GLU:O     | 3:O1:348:ILE:HG13  | 2.11                     | 0.49              |
| 4:P1:100:ALA:O     | 4:P1:103:ALA:N     | 2.45                     | 0.49              |
| 17:82:95:THR:HA    | 17:82:98:LYS:HG2   | 1.95                     | 0.49              |
| 19:A2:352:ILE:HD11 | 19:A2:528:LEU:HD22 | 1.94                     | 0.49              |
| 36:S2:189:PRO:HB2  | 36:S2:192:VAL:HG22 | 1.94                     | 0.49              |
| 56:A3:184:PHE:H    | 56:A3:256:HIS:CE1  | 2.29                     | 0.49              |
| 1:A1:15:GLN:O      | 1:A1:205:HIS:CE1   | 2.66                     | 0.49              |
| 1:A1:43:ALA:HB2    | 1:A1:189:HIS:HB3   | 1.94                     | 0.49              |
| 1:A1:385:THR:HB    | 1:A1:386:TYR:CD1   | 2.48                     | 0.49              |
| 2:B1:185:LYS:O     | 2:B1:185:LYS:CG    | 2.54                     | 0.49              |
| 2:B1:352:LEU:HD23  | 2:B1:411:ILE:CD1   | 2.43                     | 0.49              |
| 3:C1:74:ASN:O      | 5:E1:61:SER:HA     | 2.12                     | 0.49              |
| 4:D1:237:TYR:HB2   | 6:F1:60:PHE:CE1    | 2.47                     | 0.49              |
| 9:I1:70:LEU:HG     | 9:I1:72:VAL:H      | 1.78                     | 0.49              |
| 2:N1:112:LEU:O     | 2:N1:113:ARG:C     | 2.54                     | 0.49              |
| 3:O1:21:LEU:HD12   | 3:O1:22:PRO:HD2    | 1.94                     | 0.49              |
| 69:O1:401:HEM:HBC2 | 69:O1:401:HEM:CMC  | 2.35                     | 0.49              |
| 4:P1:2:ASP:HB3     | 4:P1:156:GLN:NE2   | 2.27                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:S1:34:ILE:CB     | 7:S1:35:PRO:HD3    | 2.32                     | 0.49              |
| 7:S1:48:VAL:O      | 7:S1:51:PRO:HD2    | 2.12                     | 0.49              |
| 7:S1:80:ASP:O      | 7:S1:81:ARG:HB2    | 2.11                     | 0.49              |
| 19:A2:371:VAL:HB   | 19:A2:482:GLN:HG3  | 1.94                     | 0.49              |
| 20:B2:97:LEU:CD1   | 20:B2:97:LEU:C     | 2.86                     | 0.49              |
| 20:B2:143:SER:OG   | 20:B2:147:ASN:OD1  | 2.30                     | 0.49              |
| 20:B2:266:ARG:HH22 | 23:E2:60:THR:HA    | 1.76                     | 0.49              |
| 28:J2:26:ILE:O     | 28:J2:30:SER:N     | 2.42                     | 0.49              |
| 62:G3:42:ARG:NH1   | 62:G3:74:ARG:HH21  | 2.10                     | 0.49              |
| 1:A1:146:ARG:NH2   | 1:A1:308:GLN:NE2   | 2.58                     | 0.49              |
| 2:B1:258:VAL:CG1   | 2:B1:321:LEU:HD22  | 2.42                     | 0.49              |
| 3:C1:269:LYS:CD    | 3:C1:340:GLY:HA2   | 2.43                     | 0.49              |
| 4:D1:153:PHE:O     | 4:D1:154:PRO:C     | 2.54                     | 0.49              |
| 5:E1:65:SER:O      | 5:E1:66:ALA:C      | 2.55                     | 0.49              |
| 8:H1:40:CYS:O      | 8:H1:44:VAL:HG23   | 2.12                     | 0.49              |
| 1:M1:349:ALA:O     | 1:M1:408:ARG:NH2   | 2.45                     | 0.49              |
| 2:N1:92:VAL:O      | 2:N1:92:VAL:CG1    | 2.60                     | 0.49              |
| 2:N1:170:ASN:CG    | 2:N1:171:ALA:N     | 2.70                     | 0.49              |
| 3:O1:25:SER:HB3    | 6:R1:70:MET:HE2    | 1.94                     | 0.49              |
| 3:O1:26:ASN:HA     | 6:R1:70:MET:HA     | 1.94                     | 0.49              |
| 6:R1:10:SER:HA     | 6:R1:13:LEU:CD1    | 2.42                     | 0.49              |
| 6:R1:40:ASN:CG     | 6:R1:41:ASP:H      | 2.20                     | 0.49              |
| 14:42:134:THR:O    | 14:42:142:ARG:NH1  | 2.44                     | 0.49              |
| 18:92:42:ARG:HH22  | 19:A2:199:GLY:HA3  | 1.76                     | 0.49              |
| 20:B2:86:PRO:HD3   | 20:B2:96:ARG:HA    | 1.94                     | 0.49              |
| 32:O2:50:PHE:HE1   | 32:O2:96:VAL:HG12  | 1.77                     | 0.49              |
| 51:j2:26:LEU:HA    | 51:j2:31:LEU:HD22  | 1.94                     | 0.49              |
| 63:H3:24:ASN:ND2   | 63:H3:26:THR:H     | 2.11                     | 0.49              |
| 1:A1:43:ALA:HB1    | 1:A1:189:HIS:HB3   | 1.94                     | 0.49              |
| 3:C1:200:LEU:HD13  | 69:C1:402:HEM:HAD2 | 1.93                     | 0.49              |
| 4:D1:24:THR:O      | 4:D1:25:SER:C      | 2.53                     | 0.49              |
| 4:D1:160:MET:HE2   | 4:D1:163:PRO:HG3   | 1.95                     | 0.49              |
| 1:M1:379:ILE:O     | 1:M1:383:LEU:HG    | 2.13                     | 0.49              |
| 1:M1:431:LEU:HD12  | 1:M1:432:PRO:HD2   | 1.95                     | 0.49              |
| 2:N1:255:ALA:CB    | 2:N1:426:ALA:HB2   | 2.42                     | 0.49              |
| 3:O1:4:ILE:O       | 3:O1:5:ARG:C       | 2.55                     | 0.49              |
| 3:O1:372:ILE:O     | 3:O1:375:LYS:N     | 2.45                     | 0.49              |
| 4:P1:168:VAL:HG12  | 4:P1:169:LEU:CD2   | 2.42                     | 0.49              |
| 4:P1:168:VAL:HG12  | 4:P1:169:LEU:HD23  | 1.93                     | 0.49              |
| 7:S1:71:ARG:O      | 7:S1:73:ASN:N      | 2.46                     | 0.49              |
| 19:A2:301:ARG:C    | 38:U2:137:TRP:HB2  | 2.37                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:B2:241:MET:HG3  | 39:V2:10:MET:HB3   | 1.95                     | 0.49              |
| 22:D2:155:SER:OG   | 23:E2:150:THR:O    | 2.30                     | 0.49              |
| 56:A3:145:LEU:HD21 | 58:C3:32:THR:HG21  | 1.93                     | 0.49              |
| 1:A1:53:ASN:C      | 1:A1:53:ASN:ND2    | 2.69                     | 0.49              |
| 2:B1:126:VAL:O     | 2:B1:126:VAL:HG12  | 2.11                     | 0.49              |
| 2:B1:207:ILE:HG22  | 2:B1:379:LEU:HD12  | 1.95                     | 0.49              |
| 2:B1:299:VAL:HG13  | 2:B1:303:VAL:HG21  | 1.94                     | 0.49              |
| 3:C1:103:TYR:OH    | 3:C1:322:GLN:HG3   | 2.12                     | 0.49              |
| 3:C1:119:LEU:HG    | 69:C1:402:HEM:HBB2 | 1.90                     | 0.49              |
| 3:C1:122:THR:HG21  | 3:C1:189:ILE:CG1   | 2.42                     | 0.49              |
| 4:D1:69:GLU:HG3    | 4:D1:84:PRO:HA     | 1.94                     | 0.49              |
| 4:D1:229:VAL:HG12  | 4:D1:233:ARG:NE    | 2.22                     | 0.49              |
| 2:N1:24:LEU:HD13   | 2:N1:392:TYR:CD2   | 2.48                     | 0.49              |
| 2:N1:68:LEU:CD1    | 2:N1:140:LEU:HD23  | 2.39                     | 0.49              |
| 5:Q1:38:LEU:O      | 5:Q1:42:THR:OG1    | 2.30                     | 0.49              |
| 5:Q1:42:THR:O      | 5:Q1:45:VAL:N      | 2.45                     | 0.49              |
| 5:Q1:89:PHE:O      | 5:Q1:96:LEU:N      | 2.23                     | 0.49              |
| 12:22:78:LEU:HD11  | 15:52:48:ILE:HD11  | 1.93                     | 0.49              |
| 13:32:93:PHE:HA    | 13:32:96:ILE:HD12  | 1.95                     | 0.49              |
| 35:R2:178:SER:H    | 35:R2:181:LEU:HB3  | 1.78                     | 0.49              |
| 56:A3:508:PRO:HG3  | 58:C3:6:HIS:HB3    | 1.94                     | 0.49              |
| 1:A1:37:VAL:HG13   | 1:A1:199:ALA:HB2   | 1.93                     | 0.49              |
| 1:A1:37:VAL:CG1    | 1:A1:199:ALA:HB2   | 2.43                     | 0.49              |
| 1:A1:315:ALA:HB3   | 1:A1:316:ASP:OD1   | 2.13                     | 0.49              |
| 2:B1:79:GLY:CA     | 2:B1:125:ASN:HD21  | 2.26                     | 0.49              |
| 2:B1:166:ALA:HB2   | 2:B1:244:ILE:CG1   | 2.39                     | 0.49              |
| 2:B1:183:ILE:HG22  | 2:B1:184:GLY:N     | 2.28                     | 0.49              |
| 2:B1:348:ALA:HB3   | 2:B1:418:VAL:HG21  | 1.94                     | 0.49              |
| 2:B1:381:GLU:OE1   | 2:B1:381:GLU:HA    | 2.13                     | 0.49              |
| 4:D1:13:SER:O      | 4:D1:19:SER:HB3    | 2.11                     | 0.49              |
| 4:D1:161:ALA:HB1   | 4:D1:162:PRO:HD2   | 1.93                     | 0.49              |
| 1:M1:327:ASP:OD1   | 1:M1:328:HIS:N     | 2.44                     | 0.49              |
| 1:M1:386:TYR:N     | 1:M1:386:TYR:CD1   | 2.74                     | 0.49              |
| 5:Q1:142:LEU:HD12  | 5:Q1:161:HIS:CE1   | 2.46                     | 0.49              |
| 8:T1:73:LEU:HD23   | 8:T1:73:LEU:C      | 2.37                     | 0.49              |
| 14:42:66:LEU:O     | 14:42:69:THR:OG1   | 2.28                     | 0.49              |
| 15:52:36:MET:O     | 15:52:39:SER:OG    | 2.31                     | 0.49              |
| 18:92:137:THR:O    | 18:92:141:MET:N    | 2.43                     | 0.49              |
| 19:A2:312:GLY:N    | 38:U2:144:TYR:N    | 2.61                     | 0.49              |
| 19:A2:355:LYS:HD2  | 19:A2:530:TYR:HE1  | 1.77                     | 0.49              |
| 19:A2:674:LEU:CD1  | 29:K2:46:LYS:HE2   | 2.32                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:B2:85:GLY:C     | 20:B2:87:GLN:N     | 2.70                     | 0.49              |
| 39:V2:134:LEU:HG   | 39:V2:138:TYR:HD2  | 1.78                     | 0.49              |
| 56:A3:87:ILE:O     | 56:A3:173:PRO:HD3  | 2.13                     | 0.49              |
| 62:G3:44:ARG:HD2   | 62:G3:74:ARG:O     | 2.12                     | 0.49              |
| 1:A1:286:GLY:O     | 1:A1:287:GLY:O     | 2.30                     | 0.49              |
| 1:A1:417:ASP:CG    | 10:J1:10:TYR:OH    | 2.55                     | 0.49              |
| 2:B1:207:ILE:CG2   | 2:B1:379:LEU:HD12  | 2.43                     | 0.49              |
| 2:B1:429:ASN:ND2   | 2:N1:60:SER:CB     | 2.59                     | 0.49              |
| 3:C1:88:SER:HB3    | 3:C1:250:LEU:HD21  | 1.95                     | 0.49              |
| 3:C1:210:GLY:HA3   | 3:C1:314:SER:CB    | 2.40                     | 0.49              |
| 4:D1:116:ILE:HD11  | 4:D1:120:ARG:HH11  | 1.78                     | 0.49              |
| 4:D1:139:THR:CG2   | 8:H1:44:VAL:HB     | 2.43                     | 0.49              |
| 4:D1:237:TYR:CD2   | 4:D1:239:PRO:HD3   | 2.48                     | 0.49              |
| 6:F1:73:GLN:HG2    | 7:G1:36:ASN:HD21   | 1.77                     | 0.49              |
| 1:M1:89:TYR:CD1    | 1:M1:89:TYR:C      | 2.91                     | 0.49              |
| 1:M1:262:TRP:CE3   | 1:M1:385:THR:HG21  | 2.48                     | 0.49              |
| 1:M1:286:GLY:O     | 1:M1:287:GLY:C     | 2.56                     | 0.49              |
| 2:N1:254:HIS:O     | 2:N1:426:ALA:HA    | 2.13                     | 0.49              |
| 3:O1:142:GLY:O     | 3:O1:146:ILE:HG12  | 2.12                     | 0.49              |
| 3:O1:150:LEU:O     | 3:O1:153:ILE:HD13  | 2.13                     | 0.49              |
| 3:O1:192:ILE:N     | 3:O1:192:ILE:HD13  | 2.28                     | 0.49              |
| 3:O1:329:VAL:HA    | 3:O1:332:LEU:HD12  | 1.94                     | 0.49              |
| 5:Q1:107:ASP:O     | 5:Q1:108:GLN:C     | 2.55                     | 0.49              |
| 5:Q1:188:THR:HG21  | 5:Q1:194:ILE:CD1   | 2.42                     | 0.49              |
| 19:A2:246:ARG:HH22 | 21:C2:234:LYS:H    | 1.60                     | 0.49              |
| 35:R2:329:LEU:HD11 | 35:R2:331:HIS:HD2  | 1.77                     | 0.49              |
| 39:V2:95:ALA:HB2   | 39:V2:106:VAL:HG11 | 1.95                     | 0.49              |
| 57:B3:13:THR:HG22  | 57:B3:13:THR:O     | 2.11                     | 0.49              |
| 1:A1:415:PHE:O     | 1:A1:441:MET:HE2   | 2.13                     | 0.49              |
| 2:B1:213:HIS:O     | 2:B1:213:HIS:HD2   | 1.96                     | 0.49              |
| 4:D1:138:PRO:HB3   | 8:H1:55:THR:CA     | 2.43                     | 0.49              |
| 4:D1:158:ILE:HG13  | 70:D1:301:HEC:HBD2 | 1.95                     | 0.49              |
| 4:D1:217:PRO:HG2   | 4:D1:218:LEU:H     | 1.78                     | 0.49              |
| 6:F1:45:GLU:O      | 6:F1:46:ALA:O      | 2.31                     | 0.49              |
| 1:M1:307:PHE:C     | 1:M1:307:PHE:CD1   | 2.91                     | 0.49              |
| 1:M1:370:ASP:OD1   | 2:N1:375:SER:HB3   | 2.12                     | 0.49              |
| 2:N1:227:ARG:HD2   | 2:N1:227:ARG:N     | 2.27                     | 0.49              |
| 2:N1:267:ALA:O     | 2:N1:268:GLU:C     | 2.56                     | 0.49              |
| 3:O1:221:HIS:N     | 3:O1:222:PRO:HD2   | 2.28                     | 0.49              |
| 3:O1:341:GLN:O     | 3:O1:342:PRO:C     | 2.55                     | 0.49              |
| 4:P1:49:ARG:HG3    | 4:P1:49:ARG:O      | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:T1:15:ASP:CB     | 8:T1:16:PRO:CD     | 2.91                     | 0.49              |
| 18:92:163:THR:HA   | 18:92:170:THR:HA   | 1.94                     | 0.49              |
| 52:12:73:LEU:HA    | 52:12:76:ILE:HD12  | 1.95                     | 0.49              |
| 53:62:246:LEU:O    | 53:62:251:THR:OG1  | 2.31                     | 0.49              |
| 53:62:457:LEU:O    | 53:62:461:SER:N    | 2.46                     | 0.49              |
| 1:A1:260:PRO:HG3   | 1:A1:414:TYR:CZ    | 2.49                     | 0.48              |
| 1:A1:347:THR:O     | 11:K1:16:ASN:ND2   | 2.43                     | 0.48              |
| 1:A1:433:ASP:CG    | 3:C1:223:TYR:HH    | 2.14                     | 0.48              |
| 2:B1:294:SER:O     | 2:B1:295:LEU:C     | 2.55                     | 0.48              |
| 2:B1:322:PHE:CD1   | 2:B1:322:PHE:C     | 2.90                     | 0.48              |
| 3:C1:213:SER:O     | 3:C1:214:ASP:C     | 2.56                     | 0.48              |
| 4:D1:10:TYR:CZ     | 4:D1:128:PHE:CE2   | 2.92                     | 0.48              |
| 4:D1:30:PHE:O      | 4:D1:31:GLN:C      | 2.53                     | 0.48              |
| 4:D1:32:VAL:CB     | 4:D1:186:VAL:HG22  | 2.43                     | 0.48              |
| 4:D1:134:TYR:HE2   | 4:D1:163:PRO:CG    | 2.24                     | 0.48              |
| 4:D1:138:PRO:HB3   | 8:H1:54:CYS:C      | 2.37                     | 0.48              |
| 7:G1:56:TYR:O      | 7:G1:57:LEU:C      | 2.56                     | 0.48              |
| 7:G1:80:ASP:CG     | 8:H1:47:ARG:HH22   | 2.21                     | 0.48              |
| 1:M1:243:HIS:CD2   | 1:M1:425:PHE:CE1   | 3.01                     | 0.48              |
| 1:M1:291:SER:HB3   | 2:N1:87:ARG:HD3    | 1.94                     | 0.48              |
| 1:M1:436:ARG:HE    | 3:O1:222:PRO:CD    | 2.26                     | 0.48              |
| 2:N1:72:ALA:HB2    | 2:N1:140:LEU:CD2   | 2.43                     | 0.48              |
| 2:N1:283:PRO:HG3   | 9:U1:55:LEU:HB3    | 1.95                     | 0.48              |
| 2:N1:312:PHE:HD1   | 9:U1:58:GLN:O      | 1.96                     | 0.48              |
| 3:O1:284:ILE:CG2   | 3:O1:285:PRO:HD2   | 2.43                     | 0.48              |
| 10:V1:61:ASN:O     | 10:V1:62:LYS:HB2   | 2.13                     | 0.48              |
| 12:22:149:ILE:HD12 | 12:22:154:ILE:HG21 | 1.95                     | 0.48              |
| 18:92:228:ALA:HA   | 18:92:231:LEU:HD23 | 1.94                     | 0.48              |
| 19:A2:381:LEU:HB2  | 29:K2:55:ILE:CD1   | 2.42                     | 0.48              |
| 19:A2:443:ASP:OD1  | 19:A2:443:ASP:N    | 2.45                     | 0.48              |
| 22:D2:151:VAL:HG22 | 22:D2:181:ILE:HB   | 1.95                     | 0.48              |
| 27:I2:106:GLU:HB3  | 27:I2:108:LYS:HZ1  | 1.78                     | 0.48              |
| 37:T2:21:LYS:HG2   | 37:T2:75:CYS:HB3   | 1.94                     | 0.48              |
| 53:62:381:THR:HA   | 53:62:420:ALA:HA   | 1.95                     | 0.48              |
| 57:B3:90:ILE:HD12  | 57:B3:90:ILE:H     | 1.77                     | 0.48              |
| 2:B1:128:THR:C     | 2:B1:130:PRO:HD2   | 2.39                     | 0.48              |
| 2:B1:141:GLN:OE1   | 2:B1:141:GLN:HA    | 2.13                     | 0.48              |
| 4:D1:224:ARG:HH21  | 7:G1:27:PRO:HD2    | 1.78                     | 0.48              |
| 5:E1:32:ARG:HH12   | 7:G1:22:GLU:CD     | 2.21                     | 0.48              |
| 6:F1:51:PRO:HG3    | 2:N1:134:ARG:HH12  | 1.78                     | 0.48              |
| 7:G1:34:ILE:O      | 7:G1:38:LEU:HG     | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:J1:4:THR:HG22   | 10:J1:6:THR:H      | 1.77                     | 0.48              |
| 1:M1:4:TYR:CE1     | 2:N1:43:PRO:HB3    | 2.48                     | 0.48              |
| 4:P1:66:GLU:O      | 4:P1:69:GLU:HG2    | 2.13                     | 0.48              |
| 9:U1:51:CYS:SG     | 9:U1:53:GLU:HB3    | 2.52                     | 0.48              |
| 19:A2:59:GLN:HB3   | 21:C2:241:TRP:CZ3  | 2.49                     | 0.48              |
| 19:A2:160:VAL:C    | 27:I2:102:ASN:HD22 | 2.19                     | 0.48              |
| 31:N2:6:LYS:HE2    | 31:N2:16:VAL:HG11  | 1.95                     | 0.48              |
| 35:R2:178:SER:H    | 35:R2:182:ARG:H    | 1.61                     | 0.48              |
| 35:R2:238:GLN:HE22 | 35:R2:271:TYR:HA   | 1.77                     | 0.48              |
| 35:R2:328:ILE:CG2  | 35:R2:329:LEU:N    | 2.49                     | 0.48              |
| 56:A3:397:PHE:HB3  | 56:A3:398:PRO:HD3  | 1.95                     | 0.48              |
| 58:C3:42:LEU:HD13  | 65:J3:45:TYR:HD2   | 1.77                     | 0.48              |
| 2:B1:198:HIS:HE1   | 2:B1:233:SER:CB    | 2.19                     | 0.48              |
| 3:C1:357:LEU:O     | 3:C1:361:LEU:HG    | 2.13                     | 0.48              |
| 4:D1:20:SER:OG     | 4:D1:21:LEU:N      | 2.46                     | 0.48              |
| 4:D1:102:ARG:HE    | 4:D1:109:LEU:HB2   | 1.78                     | 0.48              |
| 1:M1:161:THR:HB    | 1:M1:162:PRO:CD    | 2.41                     | 0.48              |
| 1:M1:349:ALA:HB3   | 1:M1:408:ARG:HE    | 1.78                     | 0.48              |
| 2:N1:79:GLY:H      | 2:N1:125:ASN:ND2   | 2.12                     | 0.48              |
| 2:N1:271:ALA:O     | 2:N1:272:PHE:C     | 2.57                     | 0.48              |
| 3:O1:126:THR:HG21  | 69:O1:401:HEM:CAB  | 2.43                     | 0.48              |
| 3:O1:218:ILE:HG23  | 3:O1:223:TYR:CE2   | 2.48                     | 0.48              |
| 4:P1:74:PRO:O      | 4:P1:79:GLU:N      | 2.42                     | 0.48              |
| 4:P1:178:THR:O     | 4:P1:179:MET:C     | 2.55                     | 0.48              |
| 10:V1:38:GLY:O     | 10:V1:42:ILE:HG13  | 2.14                     | 0.48              |
| 19:A2:337:ASP:O    | 19:A2:543:LYS:N    | 2.42                     | 0.48              |
| 53:62:491:LEU:O    | 53:62:494:THR:OG1  | 2.26                     | 0.48              |
| 1:A1:433:ASP:O     | 1:A1:434:TYR:C     | 2.56                     | 0.48              |
| 2:B1:132:PHE:HB3   | 2:B1:137:VAL:CG2   | 2.42                     | 0.48              |
| 2:B1:187:THR:HG23  | 2:B1:190:GLU:OE1   | 2.13                     | 0.48              |
| 4:D1:26:ILE:HG22   | 4:D1:27:ARG:N      | 2.27                     | 0.48              |
| 4:D1:131:LEU:HD22  | 4:D1:163:PRO:HB3   | 1.95                     | 0.48              |
| 4:D1:165:TYR:H     | 4:D1:168:VAL:CG2   | 2.26                     | 0.48              |
| 8:H1:62:LEU:O      | 8:H1:65:ARG:HG2    | 2.14                     | 0.48              |
| 1:M1:62:LEU:HB3    | 1:M1:122:LEU:HD22  | 1.94                     | 0.48              |
| 1:M1:80:GLU:O      | 1:M1:82:MET:N      | 2.46                     | 0.48              |
| 1:M1:100:LYS:HD2   | 1:M1:373:THR:OG1   | 2.13                     | 0.48              |
| 1:M1:280:TYR:O     | 1:M1:306:SER:HA    | 2.14                     | 0.48              |
| 1:M1:329:MET:CA    | 1:M1:329:MET:HE3   | 2.44                     | 0.48              |
| 1:M1:385:THR:CG2   | 1:M1:386:TYR:CD1   | 2.96                     | 0.48              |
| 2:N1:381:GLU:OE1   | 2:N1:381:GLU:HA    | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:233:LEU:CD2   | 4:P1:219:VAL:HG21  | 2.44                     | 0.48              |
| 12:22:122:ILE:HD13 | 12:22:128:LEU:HD11 | 1.95                     | 0.48              |
| 17:82:381:GLN:O    | 19:A2:74:ASN:O     | 2.31                     | 0.48              |
| 23:E2:61:LEU:HD23  | 39:V2:36:PHE:HE1   | 1.77                     | 0.48              |
| 23:E2:80:GLU:O     | 33:P2:25:GLN:NE2   | 2.47                     | 0.48              |
| 1:A1:239:SER:HB2   | 7:G1:18:LEU:HD23   | 1.95                     | 0.48              |
| 3:C1:175:LEU:HG    | 3:C1:175:LEU:O     | 2.11                     | 0.48              |
| 4:D1:3:LEU:HD21    | 7:G1:71:ARG:HA     | 1.95                     | 0.48              |
| 4:D1:26:ILE:O      | 4:D1:27:ARG:C      | 2.56                     | 0.48              |
| 4:D1:50:HIS:CE1    | 4:D1:91:PHE:HZ     | 2.31                     | 0.48              |
| 1:M1:277:ILE:H     | 1:M1:277:ILE:HG12  | 1.42                     | 0.48              |
| 1:M1:290:LEU:HD13  | 1:M1:295:ALA:HB1   | 1.95                     | 0.48              |
| 5:Q1:33:LYS:HB2    | 10:V1:10:TYR:CE1   | 2.48                     | 0.48              |
| 5:Q1:76:ILE:HG22   | 5:Q1:193:VAL:O     | 2.12                     | 0.48              |
| 19:A2:313:LEU:N    | 38:U2:142:THR:C    | 2.70                     | 0.48              |
| 23:E2:100:GLU:O    | 23:E2:170:GLY:N    | 2.46                     | 0.48              |
| 49:h2:121:GLU:OE2  | 49:h2:124:ARG:NH2  | 2.46                     | 0.48              |
| 64:I3:39:VAL:O     | 64:I3:42:LYS:HE2   | 2.14                     | 0.48              |
| 65:J3:8:LYS:NZ     | 65:J3:8:LYS:HB3    | 2.29                     | 0.48              |
| 1:A1:61:HIS:CE1    | 1:A1:134:ILE:HD11  | 2.49                     | 0.48              |
| 2:B1:130:PRO:HB2   | 2:B1:132:PHE:CE1   | 2.48                     | 0.48              |
| 2:B1:341:TYR:O     | 2:B1:342:ASN:C     | 2.57                     | 0.48              |
| 3:C1:218:ILE:CG2   | 3:C1:223:TYR:CE2   | 2.97                     | 0.48              |
| 4:D1:7:PRO:CB      | 4:D1:125:ASP:HB3   | 2.43                     | 0.48              |
| 9:I1:60:ALA:HB3    | 9:I1:63:PRO:O      | 2.12                     | 0.48              |
| 1:M1:329:MET:HA    | 1:M1:329:MET:HE3   | 1.95                     | 0.48              |
| 1:M1:395:TRP:O     | 1:M1:396:GLU:C     | 2.57                     | 0.48              |
| 3:O1:248:ASP:CG    | 4:P1:118:ARG:HH21  | 2.22                     | 0.48              |
| 3:O1:252:ASP:CB    | 3:O1:253:PRO:HD3   | 2.34                     | 0.48              |
| 4:P1:10:TYR:CE1    | 8:T1:73:LEU:HD22   | 2.47                     | 0.48              |
| 13:32:19:ILE:HA    | 13:32:23:TRP:HB2   | 1.96                     | 0.48              |
| 34:Q2:8:PRO:O      | 39:V2:88:ARG:NH2   | 2.46                     | 0.48              |
| 34:Q2:38:LYS:HG3   | 34:Q2:39:PRO:HD3   | 1.95                     | 0.48              |
| 1:A1:277:ILE:CG2   | 1:A1:294:LEU:HD12  | 2.44                     | 0.48              |
| 2:B1:139:ALA:O     | 2:B1:142:PRO:HD2   | 2.14                     | 0.48              |
| 3:C1:24:PRO:O      | 3:C1:224:TYR:OH    | 2.20                     | 0.48              |
| 5:E1:72:SER:HB2    | 3:O1:168:PHE:CE2   | 2.48                     | 0.48              |
| 6:F1:46:ALA:O      | 6:F1:47:ILE:C      | 2.56                     | 0.48              |
| 7:G1:50:PRO:HB2    | 7:G1:51:PRO:CD     | 2.38                     | 0.48              |
| 1:M1:33:PRO:O      | 1:M1:103:SER:HB3   | 2.14                     | 0.48              |
| 1:M1:64:PHE:HA     | 1:M1:75:LEU:HD23   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:343:MET:HE1   | 1:M1:416:TYR:CE2   | 2.47                     | 0.48              |
| 2:N1:128:THR:HG23  | 2:N1:226:ILE:HD11  | 1.96                     | 0.48              |
| 2:N1:360:ALA:O     | 2:N1:363:LYS:N     | 2.46                     | 0.48              |
| 5:Q1:96:LEU:CD2    | 5:Q1:195:VAL:HG21  | 2.27                     | 0.48              |
| 19:A2:318:THR:HG22 | 19:A2:320:GLU:H    | 1.79                     | 0.48              |
| 19:A2:542:PRO:HG2  | 19:A2:545:LEU:HD11 | 1.95                     | 0.48              |
| 20:B2:131:GLN:HE21 | 23:E2:124:PRO:HA   | 1.77                     | 0.48              |
| 22:D2:114:ARG:CG   | 22:D2:114:ARG:NH2  | 2.73                     | 0.48              |
| 35:R2:147:LYS:O    | 35:R2:151:ALA:N    | 2.47                     | 0.48              |
| 36:S2:61:LEU:HD22  | 36:S2:251:ALA:HB2  | 1.96                     | 0.48              |
| 56:A3:11:ASN:ND2   | 56:A3:13:LYS:HB2   | 2.28                     | 0.48              |
| 56:A3:266:GLU:HB2  | 56:A3:267:PRO:HD2  | 1.94                     | 0.48              |
| 59:D3:68:PHE:HA    | 59:D3:71:MET:HG2   | 1.95                     | 0.48              |
| 62:G3:42:ARG:HD2   | 62:G3:42:ARG:O     | 2.13                     | 0.48              |
| 2:B1:76:THR:HG21   | 2:B1:133:ARG:NH2   | 2.29                     | 0.48              |
| 2:B1:140:LEU:O     | 2:B1:142:PRO:N     | 2.47                     | 0.48              |
| 3:C1:108:THR:O     | 3:C1:110:LEU:N     | 2.46                     | 0.48              |
| 3:C1:297:SER:O     | 3:C1:300:ILE:CG2   | 2.62                     | 0.48              |
| 3:C1:310:SER:HB3   | 3:C1:318:ARG:HH12  | 1.71                     | 0.48              |
| 1:M1:406:VAL:O     | 1:M1:410:VAL:HG23  | 2.13                     | 0.48              |
| 2:N1:132:PHE:CE2   | 2:N1:191:LEU:HD22  | 2.49                     | 0.48              |
| 2:N1:362:ASN:O     | 2:N1:363:LYS:C     | 2.57                     | 0.48              |
| 3:O1:51:LEU:HD21   | 3:O1:79:ILE:HG22   | 1.95                     | 0.48              |
| 3:O1:300:ILE:HD13  | 3:O1:362:ILE:HG21  | 1.95                     | 0.48              |
| 3:O1:361:LEU:HD23  | 3:O1:365:LEU:CD1   | 2.36                     | 0.48              |
| 4:P1:137:PRO:HA    | 4:P1:138:PRO:HD3   | 1.58                     | 0.48              |
| 4:P1:146:GLY:O     | 4:P1:148:TYR:HD1   | 1.97                     | 0.48              |
| 5:Q1:105:GLU:O     | 5:Q1:108:GLN:HB3   | 2.14                     | 0.48              |
| 10:V1:32:GLU:HG2   | 10:V1:33:ARG:N     | 2.29                     | 0.48              |
| 17:82:257:ARG:HA   | 18:92:243:PHE:HB2  | 1.96                     | 0.48              |
| 19:A2:373:PRO:HG3  | 19:A2:486:GLY:HA3  | 1.96                     | 0.48              |
| 20:B2:97:LEU:N     | 20:B2:97:LEU:CD1   | 2.73                     | 0.48              |
| 20:B2:236:LEU:HD11 | 20:B2:241:MET:HE2  | 1.96                     | 0.48              |
| 21:C2:112:SER:HB2  | 21:C2:135:LEU:HB3  | 1.96                     | 0.48              |
| 35:R2:170:LEU:HD12 | 35:R2:328:ILE:HD12 | 1.95                     | 0.48              |
| 56:A3:507:GLU:O    | 56:A3:508:PRO:O    | 2.32                     | 0.48              |
| 1:A1:39:VAL:HG12   | 1:A1:41:ILE:HD12   | 1.95                     | 0.48              |
| 1:A1:39:VAL:HG23   | 1:A1:113:LEU:HD23  | 1.95                     | 0.48              |
| 2:B1:47:ILE:CG2    | 2:B1:48:GLY:N      | 2.77                     | 0.48              |
| 2:B1:235:ALA:O     | 2:B1:236:LYS:CB    | 2.61                     | 0.48              |
| 3:C1:147:THR:HG21  | 3:C1:165:TRP:CD1   | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:215:VAL:O     | 6:F1:63:LYS:CE     | 2.62                     | 0.48              |
| 4:D1:224:ARG:NH2   | 7:G1:27:PRO:HD2    | 2.28                     | 0.48              |
| 6:F1:73:GLN:HA     | 7:G1:39:ARG:NH2    | 2.28                     | 0.48              |
| 1:M1:134:ILE:O     | 1:M1:137:GLU:N     | 2.47                     | 0.48              |
| 1:M1:335:MET:HE3   | 1:M1:335:MET:O     | 2.14                     | 0.48              |
| 4:P1:31:GLN:O      | 4:P1:32:VAL:C      | 2.56                     | 0.48              |
| 4:P1:190:LEU:O     | 4:P1:191:ARG:C     | 2.55                     | 0.48              |
| 5:Q1:102:THR:O     | 5:Q1:105:GLU:N     | 2.46                     | 0.48              |
| 5:Q1:188:THR:HG21  | 5:Q1:194:ILE:HG13  | 1.96                     | 0.48              |
| 17:82:383:THR:HG23 | 19:A2:74:ASN:O     | 2.14                     | 0.48              |
| 19:A2:226:CYS:SG   | 75:A2:802:SF4:S1   | 3.11                     | 0.48              |
| 29:K2:67:ALA:O     | 29:K2:75:LYS:N     | 2.45                     | 0.48              |
| 40:W2:119:ILE:HD12 | 40:W2:130:ILE:HG21 | 1.95                     | 0.48              |
| 56:A3:197:LEU:O    | 58:C3:92:LEU:HD22  | 2.13                     | 0.48              |
| 57:B3:4:PRO:HB2    | 66:K3:43:SER:HA    | 1.96                     | 0.48              |
| 1:A1:84:ALA:HB1    | 1:A1:100:LYS:O     | 2.14                     | 0.48              |
| 1:A1:106:LEU:O     | 1:A1:107:PRO:C     | 2.56                     | 0.48              |
| 2:B1:303:VAL:CG1   | 2:B1:304:HIS:H     | 2.26                     | 0.48              |
| 3:C1:282:ARG:O     | 3:C1:283:SER:C     | 2.55                     | 0.48              |
| 8:H1:68:CYS:O      | 8:H1:69:VAL:C      | 2.55                     | 0.48              |
| 1:M1:236:PHE:CD2   | 1:M1:258:GLU:CG    | 2.95                     | 0.48              |
| 2:N1:24:LEU:HD13   | 2:N1:392:TYR:HD2   | 1.78                     | 0.48              |
| 2:N1:111:CYS:CB    | 2:N1:119:LEU:HD22  | 2.31                     | 0.48              |
| 3:O1:47:THR:HG21   | 3:O1:83:HIS:CB     | 2.43                     | 0.48              |
| 4:P1:153:PHE:O     | 4:P1:156:GLN:N     | 2.36                     | 0.48              |
| 5:Q1:15:ARG:HH21   | 5:Q1:32:ARG:CB     | 2.27                     | 0.48              |
| 5:Q1:29:SER:CA     | 5:Q1:32:ARG:HD3    | 2.44                     | 0.48              |
| 5:Q1:49:TYR:O      | 5:Q1:50:ALA:C      | 2.56                     | 0.48              |
| 5:Q1:87:MET:HG2    | 5:Q1:89:PHE:HE1    | 1.78                     | 0.48              |
| 5:Q1:193:VAL:O     | 5:Q1:193:VAL:CG1   | 2.61                     | 0.48              |
| 7:S1:39:ARG:HA     | 7:S1:42:ARG:HD2    | 1.96                     | 0.48              |
| 19:A2:129:PRO:HB2  | 27:I2:114:TYR:CE1  | 2.48                     | 0.48              |
| 56:A3:476:PHE:CD1  | 67:L3:15:VAL:HG21  | 2.48                     | 0.48              |
| 58:C3:80:ARG:O     | 58:C3:84:ILE:HG12  | 2.14                     | 0.48              |
| 4:D1:117:VAL:CG1   | 4:D1:191:ARG:HH11  | 2.27                     | 0.47              |
| 4:D1:232:SER:CB    | 7:G1:23:GLN:OE1    | 2.62                     | 0.47              |
| 70:D1:301:HEC:HBD1 | 70:D1:301:HEC:HHA  | 1.95                     | 0.47              |
| 7:G1:67:GLU:O      | 7:G1:71:ARG:HB3    | 2.14                     | 0.47              |
| 8:H1:15:ASP:HB2    | 8:H1:16:PRO:CD     | 2.44                     | 0.47              |
| 1:M1:53:ASN:ND2    | 1:M1:165:GLN:HG3   | 2.29                     | 0.47              |
| 2:N1:194:TYR:O     | 2:N1:195:VAL:C     | 2.55                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N1:250:ASP:OD1   | 2:N1:251:SER:N     | 2.47                     | 0.47              |
| 2:N1:262:ALA:HB3   | 2:N1:269:ALA:CA    | 2.44                     | 0.47              |
| 3:O1:315:MET:O     | 3:O1:318:ARG:N     | 2.40                     | 0.47              |
| 5:Q1:127:VAL:CG1   | 5:Q1:133:VAL:HG23  | 2.44                     | 0.47              |
| 6:R1:7:SER:O       | 6:R1:11:ARG:HD2    | 2.13                     | 0.47              |
| 17:82:364:VAL:HG12 | 17:82:400:VAL:HG22 | 1.95                     | 0.47              |
| 20:B2:207:ARG:HD3  | 22:D2:98:HIS:HE1   | 1.79                     | 0.47              |
| 44:a2:79:ASN:ND2   | 55:e2:76:PRO:HG3   | 2.29                     | 0.47              |
| 47:d2:25:PHE:HZ    | 47:d2:42:THR:C     | 2.21                     | 0.47              |
| 48:f2:58:VAL:HG12  | 48:f2:62:GLN:HG2   | 1.95                     | 0.47              |
| 52:12:169:GLN:HE21 | 52:12:174:LEU:HD13 | 1.79                     | 0.47              |
| 54:g2:70:ARG:HH22  | 54:g2:94:ARG:HD2   | 1.79                     | 0.47              |
| 40:M2:34:SER:HB3   | 40:M2:40:LEU:HD22  | 1.95                     | 0.47              |
| 58:C3:173:PHE:C    | 58:C3:173:PHE:CD1  | 2.92                     | 0.47              |
| 3:C1:77:TRP:CE3    | 3:C1:78:ILE:HG23   | 2.44                     | 0.47              |
| 4:D1:36:VAL:HG23   | 4:D1:169:LEU:HD11  | 1.96                     | 0.47              |
| 5:E1:40:THR:HG22   | 10:J1:20:PHE:HZ    | 1.79                     | 0.47              |
| 1:M1:24:ARG:CG     | 1:M1:196:VAL:HG22  | 2.45                     | 0.47              |
| 1:M1:62:LEU:O      | 1:M1:63:ALA:C      | 2.57                     | 0.47              |
| 1:M1:392:LEU:HA    | 1:M1:395:TRP:HD1   | 1.72                     | 0.47              |
| 2:N1:346:THR:HG23  | 2:N1:351:ASN:HB3   | 1.96                     | 0.47              |
| 3:O1:227:LYS:HG2   | 4:P1:223:LYS:HZ3   | 1.79                     | 0.47              |
| 5:Q1:18:VAL:HG21   | 7:S1:22:GLU:OE1    | 2.14                     | 0.47              |
| 17:82:220:GLN:OE1  | 19:A2:197:THR:OG1  | 2.32                     | 0.47              |
| 18:92:42:ARG:HH22  | 19:A2:199:GLY:CA   | 2.26                     | 0.47              |
| 19:A2:238:PHE:HB3  | 23:E2:140:ARG:CB   | 2.42                     | 0.47              |
| 19:A2:409:PHE:HD1  | 19:A2:694:PHE:HB2  | 1.79                     | 0.47              |
| 19:A2:462:PHE:O    | 19:A2:464:GLN:N    | 2.39                     | 0.47              |
| 34:Q2:5:VAL:N      | 39:V2:107:GLY:O    | 2.47                     | 0.47              |
| 53:62:202:PHE:HZ   | 53:62:263:PHE:HA   | 1.78                     | 0.47              |
| 53:62:362:LEU:HB3  | 53:62:431:LEU:HB3  | 1.96                     | 0.47              |
| 56:A3:115:SER:O    | 56:A3:121:GLY:HA2  | 2.14                     | 0.47              |
| 57:B3:16:ILE:HD12  | 57:B3:17:MET:H     | 1.78                     | 0.47              |
| 58:C3:65:SER:HB3   | 58:C3:71:HIS:CE1   | 2.48                     | 0.47              |
| 1:A1:85:HIS:CE1    | 2:B1:284:HIS:ND1   | 2.82                     | 0.47              |
| 2:B1:207:ILE:CD1   | 2:B1:383:GLY:HA2   | 2.37                     | 0.47              |
| 2:B1:242:GLY:H     | 2:B1:423:SER:HB3   | 1.80                     | 0.47              |
| 3:C1:44:GLN:HE22   | 3:C1:86:GLY:HA3    | 1.78                     | 0.47              |
| 4:D1:241:LYS:HE3   | 6:F1:53:ASN:HB3    | 1.96                     | 0.47              |
| 10:J1:13:LEU:O     | 10:J1:19:THR:OG1   | 2.16                     | 0.47              |
| 3:O1:153:ILE:CG2   | 3:O1:154:PRO:HD2   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Q1:122:HIS:ND1  | 5:Q1:124:LEU:HB2   | 2.29                     | 0.47              |
| 5:Q1:170:ARG:O    | 5:Q1:172:ARG:HG2   | 2.15                     | 0.47              |
| 57:B3:22:HIS:CE1  | 64:I3:44:LYS:HD3   | 2.49                     | 0.47              |
| 57:B3:59:GLN:O    | 57:B3:62:GLU:HB2   | 2.13                     | 0.47              |
| 1:A1:70:ARG:HB3   | 1:A1:74:ALA:HB3    | 1.97                     | 0.47              |
| 1:A1:261:GLY:HA2  | 1:A1:314:TYR:O     | 2.13                     | 0.47              |
| 1:A1:289:HIS:O    | 1:A1:290:LEU:C     | 2.55                     | 0.47              |
| 1:A1:365:LEU:HG   | 1:A1:365:LEU:O     | 2.15                     | 0.47              |
| 2:B1:76:THR:HG21  | 2:B1:133:ARG:CZ    | 2.44                     | 0.47              |
| 2:B1:218:GLN:O    | 2:B1:221:GLU:HB2   | 2.15                     | 0.47              |
| 3:C1:26:ASN:N     | 6:F1:70:MET:HB2    | 2.28                     | 0.47              |
| 3:C1:183:PHE:O    | 3:C1:183:PHE:HD1   | 1.94                     | 0.47              |
| 4:D1:23:HIS:NE2   | 10:J1:51:LEU:HA    | 2.29                     | 0.47              |
| 4:D1:137:PRO:HA   | 4:D1:138:PRO:HD3   | 1.44                     | 0.47              |
| 2:N1:24:LEU:HD12  | 2:N1:24:LEU:N      | 2.21                     | 0.47              |
| 2:N1:84:LYS:O     | 2:N1:85:ILE:C      | 2.56                     | 0.47              |
| 2:N1:299:VAL:O    | 2:N1:303:VAL:HG23  | 2.14                     | 0.47              |
| 2:N1:338:LYS:O    | 2:N1:339:ALA:C     | 2.58                     | 0.47              |
| 3:O1:341:GLN:NE2  | 3:O1:341:GLN:HA    | 2.29                     | 0.47              |
| 4:P1:131:LEU:HD22 | 4:P1:163:PRO:HB2   | 1.96                     | 0.47              |
| 5:Q1:122:HIS:HB3  | 5:Q1:125:GLU:HG3   | 1.97                     | 0.47              |
| 5:Q1:158:CYS:SG   | 5:Q1:160:CYS:HB2   | 2.54                     | 0.47              |
| 7:S1:56:TYR:HD1   | 7:S1:57:LEU:HD23   | 1.78                     | 0.47              |
| 10:V1:4:THR:HG22  | 10:V1:6:THR:H      | 1.80                     | 0.47              |
| 10:V1:52:TRP:CE3  | 10:V1:52:TRP:N     | 2.82                     | 0.47              |
| 19:A2:238:PHE:CG  | 23:E2:140:ARG:HB3  | 2.49                     | 0.47              |
| 20:B2:86:PRO:HG3  | 20:B2:96:ARG:CB    | 2.44                     | 0.47              |
| 34:Q2:110:CYS:O   | 34:Q2:114:LYS:N    | 2.42                     | 0.47              |
| 44:a2:86:THR:HA   | 44:a2:89:LEU:HB2   | 1.96                     | 0.47              |
| 52:12:233:MET:HA  | 52:12:236:ILE:HG22 | 1.97                     | 0.47              |
| 40:M2:37:MET:H    | 40:M2:41:GLY:H     | 1.61                     | 0.47              |
| 57:B3:83:ILE:O    | 57:B3:87:MET:HG3   | 2.14                     | 0.47              |
| 1:A1:52:ASN:HB2   | 1:A1:55:ALA:HB2    | 1.97                     | 0.47              |
| 2:B1:38:LEU:O     | 2:B1:39:GLU:C      | 2.56                     | 0.47              |
| 3:C1:185:LEU:HB3  | 3:C1:186:PRO:CD    | 2.36                     | 0.47              |
| 3:C1:284:ILE:CG2  | 3:C1:285:PRO:HD2   | 2.44                     | 0.47              |
| 3:C1:345:HIS:CB   | 3:C1:346:PRO:CD    | 2.85                     | 0.47              |
| 1:M1:255:ILE:O    | 1:M1:321:GLY:HA3   | 2.14                     | 0.47              |
| 1:M1:361:LEU:HG   | 1:M1:399:ILE:HD11  | 1.97                     | 0.47              |
| 3:O1:107:TYR:HE1  | 3:O1:305:PRO:HA    | 1.79                     | 0.47              |
| 3:O1:269:LYS:CD   | 3:O1:340:GLY:HA2   | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:276:PHE:CG    | 3:O1:277:ALA:N     | 2.82                     | 0.47              |
| 4:P1:64:LEU:O      | 4:P1:68:VAL:HG23   | 2.15                     | 0.47              |
| 4:P1:183:ALA:HA    | 4:P1:186:VAL:HG23  | 1.97                     | 0.47              |
| 5:Q1:118:ARG:HH12  | 5:Q1:173:LYS:N     | 2.11                     | 0.47              |
| 5:Q1:141:HIS:HA    | 5:Q1:177:PRO:HD3   | 1.96                     | 0.47              |
| 7:S1:80:ASP:CG     | 8:T1:47:ARG:HH22   | 2.21                     | 0.47              |
| 23:E2:40:TYR:HB3   | 23:E2:43:LEU:HD13  | 1.95                     | 0.47              |
| 34:Q2:118:VAL:HG13 | 34:Q2:120:PRO:HD3  | 1.96                     | 0.47              |
| 35:R2:352:VAL:HG13 | 35:R2:353:LEU:HD12 | 1.96                     | 0.47              |
| 57:B3:59:GLN:N     | 57:B3:62:GLU:HG3   | 2.24                     | 0.47              |
| 1:A1:405:ARG:O     | 1:A1:409:GLU:HG3   | 2.15                     | 0.47              |
| 2:B1:360:ALA:O     | 2:B1:363:LYS:HB2   | 2.14                     | 0.47              |
| 3:C1:192:ILE:N     | 3:C1:192:ILE:CD1   | 2.77                     | 0.47              |
| 3:C1:326:TRP:NE1   | 7:G1:48:VAL:HG22   | 2.29                     | 0.47              |
| 3:C1:361:LEU:CD2   | 3:C1:365:LEU:HD12  | 2.42                     | 0.47              |
| 4:D1:76:GLU:OE2    | 4:D1:93:LYS:O      | 2.33                     | 0.47              |
| 7:G1:33:GLY:O      | 7:G1:34:ILE:C      | 2.56                     | 0.47              |
| 7:G1:44:CYS:O      | 7:G1:45:ILE:C      | 2.57                     | 0.47              |
| 7:G1:45:ILE:HD12   | 7:G1:45:ILE:HA     | 1.67                     | 0.47              |
| 11:K1:18:VAL:HB    | 11:K1:19:PRO:HD3   | 1.95                     | 0.47              |
| 1:M1:34:THR:HB     | 2:N1:373:GLU:OE1   | 2.14                     | 0.47              |
| 1:M1:251:ALA:O     | 1:M1:325:VAL:HA    | 2.14                     | 0.47              |
| 1:M1:260:PRO:HG3   | 1:M1:414:TYR:CZ    | 2.50                     | 0.47              |
| 1:M1:436:ARG:HE    | 3:O1:222:PRO:HG3   | 1.79                     | 0.47              |
| 2:N1:163:LEU:HD22  | 2:N1:256:ALA:CB    | 2.45                     | 0.47              |
| 2:N1:197:ASN:HB2   | 2:N1:198:HIS:CD2   | 2.49                     | 0.47              |
| 3:O1:26:ASN:ND2    | 3:O1:26:ASN:O      | 2.48                     | 0.47              |
| 3:O1:208:PRO:O     | 3:O1:314:SER:OG    | 2.30                     | 0.47              |
| 3:O1:221:HIS:N     | 3:O1:222:PRO:CD    | 2.77                     | 0.47              |
| 4:P1:10:TYR:HD1    | 8:T1:74:PHE:CD1    | 2.32                     | 0.47              |
| 5:Q1:46:GLY:O      | 5:Q1:49:TYR:HB3    | 2.14                     | 0.47              |
| 5:Q1:121:GLN:CG    | 5:Q1:179:ASN:ND2   | 2.77                     | 0.47              |
| 5:Q1:163:SER:HA    | 5:Q1:173:LYS:O     | 2.14                     | 0.47              |
| 6:R1:103:GLU:O     | 6:R1:104:ARG:C     | 2.55                     | 0.47              |
| 15:52:79:VAL:O     | 15:52:83:ASN:N     | 2.48                     | 0.47              |
| 17:82:451:GLN:O    | 17:82:455:GLN:N    | 2.44                     | 0.47              |
| 19:A2:380:ASP:CG   | 29:K2:41:TYR:OH    | 2.58                     | 0.47              |
| 21:C2:154:PRO:HG2  | 32:O2:18:LYS:HE2   | 1.97                     | 0.47              |
| 35:R2:237:LYS:HA   | 35:R2:325:THR:HG23 | 1.96                     | 0.47              |
| 42:Y2:64:PHE:HA    | 42:Y2:67:THR:HG22  | 1.97                     | 0.47              |
| 47:d2:29:TYR:H     | 47:d2:98:ARG:HH12  | 1.61                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:B3:63:THR:O     | 57:B3:66:THR:HG22  | 2.15                     | 0.47              |
| 57:B3:108:TYR:N    | 57:B3:108:TYR:CD1  | 2.83                     | 0.47              |
| 58:C3:164:PHE:O    | 58:C3:168:THR:HG23 | 2.14                     | 0.47              |
| 1:A1:64:PHE:HE2    | 1:A1:88:ALA:CB     | 2.27                     | 0.47              |
| 1:A1:89:TYR:C      | 1:A1:89:TYR:HD1    | 2.21                     | 0.47              |
| 1:A1:131:ARG:NH2   | 1:A1:177:LEU:O     | 2.47                     | 0.47              |
| 1:A1:260:PRO:CD    | 1:A1:414:TYR:CE1   | 2.92                     | 0.47              |
| 1:A1:372:THR:O     | 1:A1:373:THR:C     | 2.58                     | 0.47              |
| 1:A1:426:GLY:CA    | 1:A1:427:PRO:C     | 2.86                     | 0.47              |
| 2:B1:52:LYS:CB     | 2:B1:203:ARG:HB3   | 2.28                     | 0.47              |
| 2:B1:83:PHE:CZ     | 2:B1:87:ARG:HG3    | 2.49                     | 0.47              |
| 2:B1:207:ILE:HG22  | 2:B1:379:LEU:CD1   | 2.44                     | 0.47              |
| 2:B1:247:GLN:NE2   | 2:B1:429:ASN:ND2   | 2.59                     | 0.47              |
| 2:B1:252:LEU:HD11  | 9:I1:49:VAL:HB     | 1.95                     | 0.47              |
| 3:C1:80:ARG:HD3    | 3:C1:80:ARG:C      | 2.39                     | 0.47              |
| 3:C1:108:THR:CB    | 3:C1:313:ARG:HH11  | 2.27                     | 0.47              |
| 4:D1:161:ALA:O     | 4:D1:163:PRO:HD3   | 2.14                     | 0.47              |
| 4:D1:220:TYR:O     | 4:D1:221:ALA:C     | 2.56                     | 0.47              |
| 5:E1:33:LYS:HA     | 7:G1:21:PHE:CD2    | 2.50                     | 0.47              |
| 6:F1:99:ARG:O      | 6:F1:100:GLU:C     | 2.57                     | 0.47              |
| 8:H1:50:THR:HG22   | 8:H1:51:GLU:N      | 2.29                     | 0.47              |
| 1:M1:61:HIS:CD2    | 2:N1:287:ARG:HD3   | 2.50                     | 0.47              |
| 2:N1:56:ARG:HH22   | 2:N1:318:ASP:CG    | 2.18                     | 0.47              |
| 3:O1:41:LEU:HD23   | 3:O1:190:MET:HG3   | 1.96                     | 0.47              |
| 3:O1:119:LEU:HD23  | 69:O1:402:HEM:C3B  | 2.49                     | 0.47              |
| 3:O1:174:THR:CG2   | 3:O1:178:PHE:HE2   | 2.12                     | 0.47              |
| 3:O1:312:GLN:NE2   | 3:O1:317:PHE:HB2   | 2.30                     | 0.47              |
| 3:O1:345:HIS:CB    | 3:O1:346:PRO:CD    | 2.88                     | 0.47              |
| 4:P1:80:MET:H      | 4:P1:80:MET:HG2    | 1.49                     | 0.47              |
| 4:P1:115:TYR:O     | 4:P1:119:ALA:N     | 2.47                     | 0.47              |
| 4:P1:220:TYR:CD2   | 7:S1:26:PHE:CE1    | 3.02                     | 0.47              |
| 6:R1:22:ASN:O      | 6:R1:23:ALA:C      | 2.57                     | 0.47              |
| 6:R1:45:GLU:O      | 6:R1:49:ARG:HG3    | 2.14                     | 0.47              |
| 12:22:252:GLY:HA3  | 12:22:290:LEU:HD13 | 1.96                     | 0.47              |
| 12:22:260:PHE:HE2  | 12:22:264:TRP:HE3  | 1.63                     | 0.47              |
| 14:42:306:PRO:HA   | 14:42:308:SER:H    | 1.80                     | 0.47              |
| 14:42:343:ILE:HA   | 14:42:413:MET:HE2  | 1.96                     | 0.47              |
| 17:82:79:GLU:O     | 17:82:82:THR:OG1   | 2.30                     | 0.47              |
| 18:92:75:LYS:O     | 18:92:77:ALA:N     | 2.45                     | 0.47              |
| 19:A2:130:ILE:HG12 | 27:I2:114:TYR:HH   | 1.77                     | 0.47              |
| 21:C2:73:LYS:NZ    | 31:N2:101:GLU:OE1  | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:I2:62:GLU:HB3   | 38:U2:124:TYR:HA   | 1.97                     | 0.47              |
| 36:S2:100:CYS:HB3  | 36:S2:119:LEU:HB2  | 1.97                     | 0.47              |
| 40:W2:97:LYS:HZ3   | 40:W2:107:ASP:CB   | 2.27                     | 0.47              |
| 40:W2:122:MET:O    | 40:W2:127:GLY:N    | 2.43                     | 0.47              |
| 52:12:21:THR:O     | 52:12:25:ARG:HG3   | 2.14                     | 0.47              |
| 52:12:287:HIS:CE1  | 52:12:291:LYS:HG3  | 2.49                     | 0.47              |
| 53:62:592:LEU:HD23 | 53:62:596:LEU:HD23 | 1.97                     | 0.47              |
| 59:D3:41:LYS:HD3   | 59:D3:62:LEU:HD23  | 1.97                     | 0.47              |
| 61:F3:49:VAL:HG21  | 61:F3:74:LEU:HD12  | 1.95                     | 0.47              |
| 65:J3:16:ASN:ND2   | 65:J3:16:ASN:H     | 2.12                     | 0.47              |
| 4:D1:32:VAL:CG2    | 4:D1:186:VAL:HG22  | 2.44                     | 0.47              |
| 8:H1:22:GLU:O      | 8:H1:23:GLN:C      | 2.57                     | 0.47              |
| 10:J1:32:GLU:HG2   | 10:J1:33:ARG:H     | 1.79                     | 0.47              |
| 10:J1:51:LEU:O     | 10:J1:54:HIS:N     | 2.46                     | 0.47              |
| 10:J1:55:ILE:O     | 10:J1:58:LYS:HD2   | 2.14                     | 0.47              |
| 2:N1:360:ALA:O     | 2:N1:361:LYS:C     | 2.58                     | 0.47              |
| 3:O1:9:PRO:HB2     | 3:O1:12:LYS:HB2    | 1.96                     | 0.47              |
| 3:O1:107:TYR:CE1   | 3:O1:305:PRO:HA    | 2.50                     | 0.47              |
| 3:O1:218:ILE:CD1   | 4:P1:230:LEU:HD13  | 2.45                     | 0.47              |
| 4:P1:188:THR:O     | 4:P1:189:PHE:C     | 2.55                     | 0.47              |
| 5:Q1:122:HIS:CE1   | 5:Q1:124:LEU:HD12  | 2.50                     | 0.47              |
| 5:Q1:141:HIS:HE2   | 5:Q1:175:PRO:HB2   | 1.78                     | 0.47              |
| 19:A2:97:MET:HB2   | 19:A2:100:TRP:HE1  | 1.79                     | 0.47              |
| 19:A2:427:LEU:H    | 25:G2:169:ARG:NH2  | 2.12                     | 0.47              |
| 20:B2:82:LEU:HD11  | 52:12:126:LYS:CG   | 2.44                     | 0.47              |
| 35:R2:114:ASP:HA   | 35:R2:117:ARG:HB2  | 1.95                     | 0.47              |
| 37:T2:94:GLY:HA3   | 37:T2:119:GLY:HA2  | 1.96                     | 0.47              |
| 45:b2:100:GLU:H    | 45:b2:101:ILE:HA   | 1.79                     | 0.47              |
| 1:A1:36:THR:CB     | 1:A1:372:THR:HG22  | 2.45                     | 0.47              |
| 1:A1:277:ILE:HG22  | 1:A1:294:LEU:HD12  | 1.96                     | 0.47              |
| 2:B1:227:ARG:N     | 2:B1:227:ARG:HD2   | 2.30                     | 0.47              |
| 3:C1:28:SER:CB     | 3:C1:30:TRP:HD1    | 2.28                     | 0.47              |
| 5:E1:65:SER:OG     | 5:E1:67:ASP:HB3    | 2.15                     | 0.47              |
| 11:K1:19:PRO:O     | 11:K1:23:LEU:HG    | 2.14                     | 0.47              |
| 1:M1:32:GLN:CG     | 1:M1:33:PRO:CD     | 2.86                     | 0.47              |
| 1:M1:276:ILE:O     | 1:M1:277:ILE:C     | 2.57                     | 0.47              |
| 2:N1:308:ASP:OD1   | 2:N1:308:ASP:C     | 2.57                     | 0.47              |
| 3:O1:122:THR:CG2   | 3:O1:189:ILE:HG12  | 2.44                     | 0.47              |
| 5:Q1:76:ILE:HD12   | 5:Q1:192:MET:HE1   | 1.97                     | 0.47              |
| 7:S1:68:LYS:O      | 7:S1:69:SER:C      | 2.58                     | 0.47              |
| 10:V1:52:TRP:HE3   | 10:V1:52:TRP:H     | 1.62                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:22:120:GLN:HG2  | 12:22:177:LYS:HE3  | 1.97                     | 0.47              |
| 14:42:435:ALA:O    | 14:42:438:SER:OG   | 2.31                     | 0.47              |
| 19:A2:261:ILE:HG22 | 19:A2:286:ILE:HD11 | 1.97                     | 0.47              |
| 19:A2:485:ASP:HB3  | 19:A2:680:LEU:HG   | 1.97                     | 0.47              |
| 40:M2:75:GLU:HA    | 40:M2:78:ASP:HB2   | 1.97                     | 0.47              |
| 61:F3:31:TYR:HE1   | 61:F3:98:HIS:HE1   | 1.62                     | 0.47              |
| 62:G3:67:HIS:CD2   | 62:G3:78:LEU:HD11  | 2.50                     | 0.47              |
| 2:B1:37:SER:HB3    | 2:B1:213:HIS:HB2   | 1.97                     | 0.47              |
| 2:B1:216:LEU:O     | 2:B1:217:LYS:C     | 2.57                     | 0.47              |
| 2:B1:276:GLN:OE1   | 2:B1:313:ASN:HB3   | 2.14                     | 0.47              |
| 3:C1:26:ASN:HB2    | 6:F1:69:SER:HG     | 1.70                     | 0.47              |
| 3:C1:105:GLY:HA2   | 3:C1:107:TYR:CE1   | 2.50                     | 0.47              |
| 3:C1:280:ILE:HD13  | 3:C1:280:ILE:H     | 1.80                     | 0.47              |
| 3:C1:373:GLU:HA    | 3:C1:376:LEU:HD12  | 1.97                     | 0.47              |
| 11:K1:30:VAL:HA    | 11:K1:33:VAL:CG1   | 2.44                     | 0.47              |
| 1:M1:34:THR:CB     | 2:N1:373:GLU:OE1   | 2.62                     | 0.47              |
| 1:M1:287:GLY:O     | 1:M1:289:HIS:N     | 2.48                     | 0.47              |
| 3:O1:64:SER:O      | 3:O1:65:SER:C      | 2.55                     | 0.47              |
| 3:O1:183:PHE:CE1   | 3:O1:187:PHE:CE2   | 3.03                     | 0.47              |
| 21:C2:156:GLU:HA   | 21:C2:181:ALA:HB3  | 1.96                     | 0.47              |
| 46:c2:38:GLN:HA    | 46:c2:39:ARG:HA    | 1.67                     | 0.47              |
| 59:D3:33:LEU:HD22  | 59:D3:37:GLN:HB3   | 1.97                     | 0.47              |
| 1:A1:312:ILE:HB    | 1:A1:319:LEU:HB2   | 1.97                     | 0.46              |
| 1:A1:324:PHE:CG    | 1:A1:334:MET:HG2   | 2.50                     | 0.46              |
| 2:B1:279:LEU:HD23  | 2:B1:295:LEU:HD13  | 1.94                     | 0.46              |
| 2:B1:308:ASP:OD2   | 9:I1:54:SER:O      | 2.32                     | 0.46              |
| 4:D1:138:PRO:CB    | 8:H1:55:THR:HA     | 2.46                     | 0.46              |
| 4:D1:168:VAL:HG12  | 4:D1:169:LEU:HD23  | 1.97                     | 0.46              |
| 4:D1:220:TYR:CD2   | 7:G1:26:PHE:CE1    | 3.03                     | 0.46              |
| 6:F1:36:THR:O      | 6:F1:36:THR:HG22   | 2.14                     | 0.46              |
| 7:G1:36:ASN:O      | 7:G1:37:VAL:C      | 2.56                     | 0.46              |
| 1:M1:45:SER:OG     | 1:M1:92:ARG:HG2    | 2.15                     | 0.46              |
| 1:M1:61:HIS:HB3    | 1:M1:130:GLU:HG3   | 1.97                     | 0.46              |
| 2:N1:68:LEU:HG     | 2:N1:191:LEU:HD21  | 1.98                     | 0.46              |
| 3:O1:130:GLY:HA3   | 3:O1:182:HIS:CE1   | 2.49                     | 0.46              |
| 4:P1:233:ARG:HG3   | 7:S1:17:SER:CB     | 2.42                     | 0.46              |
| 5:Q1:99:ARG:NH1    | 5:Q1:156:TYR:CZ    | 2.83                     | 0.46              |
| 5:Q1:103:LYS:HA    | 5:Q1:106:ILE:CD1   | 2.43                     | 0.46              |
| 5:Q1:114:VAL:O     | 5:Q1:117:LEU:CB    | 2.63                     | 0.46              |
| 6:R1:35:ASP:OD1    | 6:R1:89:TYR:OH     | 2.22                     | 0.46              |
| 6:R1:73:GLN:HA     | 7:S1:39:ARG:NH2    | 2.29                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:R1:88:SER:O      | 6:R1:92:PRO:HD2   | 2.15                     | 0.46              |
| 18:92:57:PRO:HA    | 18:92:60:TYR:HD2  | 1.79                     | 0.46              |
| 20:B2:322:SER:OG   | 20:B2:328:ASP:OD2 | 2.31                     | 0.46              |
| 36:S2:161:MET:HG2  | 36:S2:167:ILE:HB  | 1.98                     | 0.46              |
| 44:a2:79:ASN:ND2   | 55:e2:76:PRO:CD   | 2.73                     | 0.46              |
| 57:B3:185:MET:SD   | 57:B3:185:MET:C   | 2.99                     | 0.46              |
| 59:D3:33:LEU:HD13  | 59:D3:41:LYS:HG3  | 1.97                     | 0.46              |
| 59:D3:108:PRO:HG2  | 59:D3:111:PHE:CD2 | 2.50                     | 0.46              |
| 2:B1:84:LYS:HG3    | 2:B1:122:PHE:HZ   | 1.80                     | 0.46              |
| 2:B1:135:TRP:NE1   | 2:B1:136:GLU:HG3  | 2.31                     | 0.46              |
| 2:B1:159:VAL:HG12  | 2:B1:160:ILE:N    | 2.30                     | 0.46              |
| 3:C1:15:ASN:ND2    | 3:C1:18:PHE:HE1   | 2.12                     | 0.46              |
| 3:C1:26:ASN:ND2    | 3:C1:26:ASN:O     | 2.48                     | 0.46              |
| 3:C1:110:LEU:HG    | 3:C1:114:ASN:ND2  | 2.27                     | 0.46              |
| 11:K1:33:VAL:HG13  | 11:K1:34:TRP:CD1  | 2.50                     | 0.46              |
| 1:M1:43:ALA:HB1    | 1:M1:189:HIS:HB3  | 1.97                     | 0.46              |
| 1:M1:57:TYR:HE2    | 1:M1:134:ILE:HD12 | 1.80                     | 0.46              |
| 2:N1:262:ALA:HB2   | 2:N1:272:PHE:CE2  | 2.49                     | 0.46              |
| 3:O1:26:ASN:O      | 3:O1:27:ILE:HG13  | 2.14                     | 0.46              |
| 4:P1:30:PHE:CE1    | 4:P1:50:HIS:CE1   | 3.03                     | 0.46              |
| 5:Q1:147:ILE:O     | 5:Q1:148:ALA:C    | 2.57                     | 0.46              |
| 14:42:88:ASN:HB2   | 14:42:91:ARG:HE   | 1.80                     | 0.46              |
| 14:42:138:ASN:ND2  | 14:42:223:ALA:O   | 2.48                     | 0.46              |
| 19:A2:422:TRP:C    | 25:G2:169:ARG:CD  | 2.81                     | 0.46              |
| 19:A2:427:LEU:N    | 25:G2:169:ARG:NH1 | 2.60                     | 0.46              |
| 49:h2:147:ILE:HG22 | 49:h2:149:LEU:H   | 1.80                     | 0.46              |
| 56:A3:240:HIS:NE2  | 56:A3:244:TYR:CE2 | 2.81                     | 0.46              |
| 59:D3:102:TYR:CD2  | 68:M3:35:TYR:HE1  | 2.34                     | 0.46              |
| 1:A1:49:SER:N      | 1:A1:52:ASN:OD1   | 2.35                     | 0.46              |
| 1:A1:60:GLU:OE1    | 1:A1:90:SER:HB2   | 2.15                     | 0.46              |
| 1:A1:67:THR:CG2    | 1:A1:70:ARG:HB2   | 2.43                     | 0.46              |
| 2:B1:145:ARG:HG3   | 2:B1:183:ILE:HD13 | 1.97                     | 0.46              |
| 4:D1:165:TYR:CD1   | 4:D1:168:VAL:HG22 | 2.51                     | 0.46              |
| 6:F1:95:LYS:O      | 6:F1:96:GLU:C     | 2.57                     | 0.46              |
| 1:M1:4:TYR:O       | 1:M1:5:ALA:C      | 2.56                     | 0.46              |
| 1:M1:39:VAL:CG1    | 1:M1:41:ILE:HD11  | 2.40                     | 0.46              |
| 1:M1:241:ILE:HG13  | 7:S1:16:TYR:CD2   | 2.50                     | 0.46              |
| 1:M1:253:VAL:O     | 1:M1:323:HIS:HA   | 2.16                     | 0.46              |
| 2:N1:279:LEU:CD2   | 2:N1:295:LEU:HD13 | 2.45                     | 0.46              |
| 3:O1:248:ASP:O     | 3:O1:249:LEU:C    | 2.58                     | 0.46              |
| 3:O1:252:ASP:CB    | 3:O1:253:PRO:CD   | 2.90                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:278:TYR:O     | 3:O1:281:LEU:N     | 2.48                     | 0.46              |
| 8:T1:73:LEU:CD2    | 8:T1:74:PHE:HD1    | 2.28                     | 0.46              |
| 18:92:110:MET:HA   | 18:92:113:TYR:HD2  | 1.81                     | 0.46              |
| 18:92:111:ARG:NH2  | 19:A2:187:SER:HB2  | 2.31                     | 0.46              |
| 19:A2:312:GLY:H    | 38:U2:143:PRO:CA   | 2.28                     | 0.46              |
| 19:A2:364:ASP:OD1  | 19:A2:364:ASP:N    | 2.48                     | 0.46              |
| 26:H2:45:HIS:CE1   | 45:b2:176:LYS:H    | 2.32                     | 0.46              |
| 29:K2:35:ASP:OD1   | 29:K2:39:LYS:NZ    | 2.39                     | 0.46              |
| 52:12:127:TYR:C    | 52:12:127:TYR:HD1  | 2.23                     | 0.46              |
| 53:62:343:SER:HA   | 53:62:346:ILE:HD12 | 1.97                     | 0.46              |
| 56:A3:172:LYS:HB3  | 56:A3:176:MET:HE2  | 1.96                     | 0.46              |
| 66:K3:9:PHE:HD1    | 66:K3:10:HIS:HD2   | 1.64                     | 0.46              |
| 68:M3:1:ILE:HG23   | 68:M3:1:ILE:O      | 2.15                     | 0.46              |
| 1:A1:120:CYS:HB2   | 1:A1:122:LEU:HD21  | 1.96                     | 0.46              |
| 3:C1:8:HIS:O       | 3:C1:9:PRO:C       | 2.57                     | 0.46              |
| 3:C1:40:CYS:HB3    | 3:C1:90:PHE:HD2    | 1.81                     | 0.46              |
| 3:C1:63:PHE:O      | 3:C1:67:THR:OG1    | 2.33                     | 0.46              |
| 3:C1:252:ASP:CB    | 3:C1:253:PRO:CD    | 2.88                     | 0.46              |
| 3:C1:341:GLN:HA    | 3:C1:341:GLN:NE2   | 2.31                     | 0.46              |
| 3:C1:357:LEU:HG    | 3:C1:361:LEU:HD11  | 1.98                     | 0.46              |
| 4:D1:93:LYS:O      | 4:D1:94:PRO:C      | 2.56                     | 0.46              |
| 6:F1:45:GLU:O      | 6:F1:46:ALA:C      | 2.56                     | 0.46              |
| 1:M1:438:ARG:HG3   | 1:M1:438:ARG:NH1   | 2.31                     | 0.46              |
| 3:O1:322:GLN:HE21  | 3:O1:326:TRP:HE1   | 1.62                     | 0.46              |
| 4:P1:241:LYS:NZ    | 6:R1:53:ASN:HB2    | 2.31                     | 0.46              |
| 5:Q1:43:THR:HG22   | 5:Q1:44:THR:N      | 2.30                     | 0.46              |
| 5:Q1:133:VAL:HG13  | 5:Q1:133:VAL:O     | 2.15                     | 0.46              |
| 5:Q1:134:ILE:HD11  | 5:Q1:185:TYR:CD1   | 2.48                     | 0.46              |
| 14:42:235:LEU:HA   | 14:42:238:LEU:HG   | 1.97                     | 0.46              |
| 19:A2:111:LYS:CD   | 33:P2:53:TYR:OH    | 2.63                     | 0.46              |
| 19:A2:394:VAL:HG22 | 19:A2:473:MET:HE1  | 1.97                     | 0.46              |
| 32:O2:98:LYS:HB3   | 32:O2:102:HIS:HB2  | 1.96                     | 0.46              |
| 48:f2:40:PHE:HA    | 48:f2:43:LEU:HB3   | 1.96                     | 0.46              |
| 53:62:139:GLN:HA   | 53:62:142:ILE:HD12 | 1.98                     | 0.46              |
| 1:A1:91:THR:HG22   | 1:A1:93:GLU:N      | 2.18                     | 0.46              |
| 2:B1:141:GLN:HE22  | 2:B1:186:VAL:HB    | 1.79                     | 0.46              |
| 3:C1:310:SER:OG    | 3:C1:311:LYS:N     | 2.48                     | 0.46              |
| 3:C1:376:LEU:HD13  | 6:F1:20:TYR:CD2    | 2.51                     | 0.46              |
| 4:D1:153:PHE:O     | 4:D1:156:GLN:N     | 2.35                     | 0.46              |
| 1:M1:28:GLU:OE1    | 1:M1:375:VAL:HG11  | 2.15                     | 0.46              |
| 1:M1:70:ARG:HB3    | 1:M1:74:ALA:HB3    | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:M1:279:HIS:CE1   | 1:M1:284:TYR:OH   | 2.68                     | 0.46              |
| 2:N1:38:LEU:HD13   | 2:N1:378:PHE:CE2  | 2.50                     | 0.46              |
| 2:N1:276:GLN:OE1   | 2:N1:313:ASN:HB3  | 2.15                     | 0.46              |
| 3:O1:102:LEU:HD23  | 3:O1:102:LEU:HA   | 1.67                     | 0.46              |
| 3:O1:116:GLY:HA3   | 69:O1:402:HEM:C3C | 2.51                     | 0.46              |
| 3:O1:236:ILE:O     | 3:O1:237:LEU:C    | 2.57                     | 0.46              |
| 7:S1:34:ILE:O      | 7:S1:38:LEU:HG    | 2.14                     | 0.46              |
| 72:22:401:3PE:H2C2 | 14:42:16:TRP:HE1  | 1.80                     | 0.46              |
| 19:A2:246:ARG:NH2  | 21:C2:234:LYS:H   | 2.14                     | 0.46              |
| 39:V2:58:ARG:NH2   | 52:12:314:ILE:O   | 2.47                     | 0.46              |
| 44:a2:43:LEU:O     | 44:a2:47:TYR:N    | 2.49                     | 0.46              |
| 59:D3:23:PRO:HB3   | 60:E3:70:VAL:CG2  | 2.45                     | 0.46              |
| 1:A1:184:GLU:O     | 1:A1:188:ARG:HG3  | 2.16                     | 0.46              |
| 3:C1:152:ALA:CA    | 3:C1:287:LYS:HZ2  | 2.29                     | 0.46              |
| 7:G1:36:ASN:HA     | 7:G1:39:ARG:CD    | 2.32                     | 0.46              |
| 2:N1:286:LYS:O     | 2:N1:287:ARG:HB2  | 2.14                     | 0.46              |
| 3:O1:278:TYR:O     | 3:O1:279:ALA:C    | 2.55                     | 0.46              |
| 4:P1:240:PRO:CG    | 4:P1:241:LYS:N    | 2.79                     | 0.46              |
| 5:Q1:94:LYS:HD2    | 5:Q1:138:VAL:HG21 | 1.97                     | 0.46              |
| 7:S1:40:ARG:O      | 7:S1:44:CYS:SG    | 2.71                     | 0.46              |
| 10:V1:56:LYS:HE2   | 10:V1:60:GLU:OE1  | 2.15                     | 0.46              |
| 19:A2:351:LEU:O    | 19:A2:530:TYR:OH  | 2.34                     | 0.46              |
| 20:B2:293:LEU:O    | 20:B2:296:SER:N   | 2.35                     | 0.46              |
| 31:N2:114:TRP:O    | 31:N2:116:ILE:N   | 2.46                     | 0.46              |
| 33:P2:34:ARG:NH2   | 38:U2:92:CYS:O    | 2.46                     | 0.46              |
| 56:A3:484:THR:HB   | 68:M3:2:THR:OG1   | 2.15                     | 0.46              |
| 61:F3:98:HIS:ND1   | 61:F3:98:HIS:N    | 2.64                     | 0.46              |
| 1:A1:61:HIS:HB3    | 1:A1:130:GLU:HG3  | 1.97                     | 0.46              |
| 1:A1:91:THR:HG22   | 1:A1:92:ARG:N     | 2.31                     | 0.46              |
| 1:A1:236:PHE:CD2   | 1:A1:258:GLU:CG   | 2.92                     | 0.46              |
| 2:B1:99:THR:O      | 2:B1:99:THR:HG22  | 2.14                     | 0.46              |
| 3:C1:30:TRP:HA     | 3:C1:33:PHE:CE2   | 2.51                     | 0.46              |
| 3:C1:51:LEU:CD2    | 3:C1:79:ILE:CG2   | 2.93                     | 0.46              |
| 3:C1:246:ALA:N     | 3:C1:247:PRO:HD3  | 2.31                     | 0.46              |
| 3:C1:334:THR:O     | 3:C1:337:TRP:HB3  | 2.15                     | 0.46              |
| 4:D1:10:TYR:CE1    | 4:D1:128:PHE:HE2  | 2.34                     | 0.46              |
| 1:M1:40:TRP:CZ2    | 1:M1:377:GLU:CA   | 2.95                     | 0.46              |
| 2:N1:269:ALA:O     | 2:N1:270:ASN:C    | 2.57                     | 0.46              |
| 3:O1:277:ALA:O     | 3:O1:278:TYR:C    | 2.57                     | 0.46              |
| 4:P1:10:TYR:CZ     | 4:P1:128:PHE:CE2  | 2.92                     | 0.46              |
| 15:52:17:VAL:HA    | 15:52:20:LEU:HB3  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:Q2:86:TRP:HA    | 34:Q2:89:ILE:HG22  | 1.98                     | 0.46              |
| 35:R2:154:GLN:HG3  | 35:R2:155:VAL:H    | 1.81                     | 0.46              |
| 39:V2:20:ASP:HB2   | 39:V2:22:LYS:H     | 1.81                     | 0.46              |
| 56:A3:306:THR:HB   | 56:A3:359:ALA:O    | 2.15                     | 0.46              |
| 64:I3:19:PHE:CD1   | 64:I3:19:PHE:C     | 2.94                     | 0.46              |
| 1:A1:21:ASN:CB     | 1:A1:217:SER:HB3   | 2.45                     | 0.46              |
| 1:A1:32:GLN:HG2    | 1:A1:33:PRO:N      | 2.30                     | 0.46              |
| 1:A1:360:LEU:HD22  | 2:B1:93:GLY:HA2    | 1.97                     | 0.46              |
| 1:A1:369:LEU:HD21  | 1:A1:378:ASP:OD2   | 2.16                     | 0.46              |
| 2:B1:113:ARG:O     | 2:B1:116:VAL:HG23  | 2.15                     | 0.46              |
| 2:B1:182:ARG:NH1   | 2:B1:185:LYS:CG    | 2.77                     | 0.46              |
| 2:B1:285:VAL:O     | 2:B1:285:VAL:HG12  | 2.16                     | 0.46              |
| 3:C1:31:TRP:CD2    | 3:C1:100:ARG:HD2   | 2.50                     | 0.46              |
| 3:C1:328:LEU:O     | 3:C1:329:VAL:C     | 2.56                     | 0.46              |
| 3:C1:346:PRO:CG    | 7:G1:66:PHE:HD1    | 2.28                     | 0.46              |
| 3:C1:347:TYR:O     | 3:C1:348:ILE:C     | 2.59                     | 0.46              |
| 4:D1:10:TYR:CE1    | 8:H1:73:LEU:HD22   | 2.51                     | 0.46              |
| 4:D1:233:ARG:CG    | 7:G1:17:SER:CB     | 2.94                     | 0.46              |
| 7:G1:60:THR:O      | 7:G1:61:TRP:C      | 2.59                     | 0.46              |
| 1:M1:14:THR:HG21   | 1:M1:390:ILE:HG13  | 1.98                     | 0.46              |
| 1:M1:184:GLU:O     | 1:M1:185:TYR:C     | 2.56                     | 0.46              |
| 3:O1:61:THR:O      | 3:O1:64:SER:N      | 2.48                     | 0.46              |
| 3:O1:313:ARG:CB    | 6:R1:38:HIS:CD2    | 2.98                     | 0.46              |
| 4:P1:23:HIS:NE2    | 10:V1:51:LEU:HA    | 2.31                     | 0.46              |
| 4:P1:224:ARG:HH21  | 7:S1:27:PRO:HD2    | 1.79                     | 0.46              |
| 19:A2:157:LYS:HB2  | 27:I2:100:TYR:CD2  | 2.51                     | 0.46              |
| 19:A2:303:THR:HG23 | 38:U2:136:GLU:CA   | 2.46                     | 0.46              |
| 20:B2:92:HIS:HE1   | 20:B2:141:TYR:CE2  | 2.34                     | 0.46              |
| 23:E2:150:THR:OG1  | 23:E2:151:LYS:N    | 2.48                     | 0.46              |
| 27:I2:106:GLU:N    | 27:I2:106:GLU:CD   | 2.73                     | 0.46              |
| 40:W2:97:LYS:NZ    | 40:W2:107:ASP:CB   | 2.79                     | 0.46              |
| 48:f2:128:LEU:O    | 48:f2:132:SER:OG   | 2.34                     | 0.46              |
| 57:B3:1:MET:SD     | 57:B3:133:LEU:HD11 | 2.56                     | 0.46              |
| 59:D3:66:GLU:O     | 60:E3:66:ARG:NH2   | 2.49                     | 0.46              |
| 62:G3:5:LYS:NZ     | 62:G3:5:LYS:HB3    | 2.27                     | 0.46              |
| 1:A1:51:LYS:O      | 1:A1:53:ASN:N      | 2.46                     | 0.46              |
| 3:C1:165:TRP:HA    | 3:C1:174:THR:OG1   | 2.15                     | 0.46              |
| 3:C1:378:LYS:NZ    | 6:F1:91:GLU:OE1    | 2.48                     | 0.46              |
| 4:D1:195:GLU:HG3   | 4:D1:195:GLU:O     | 2.15                     | 0.46              |
| 1:M1:11:VAL:CG1    | 1:M1:12:PRO:HD2    | 2.46                     | 0.46              |
| 1:M1:192:ALA:HA    | 1:M1:194:ARG:N     | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M1:243:HIS:O    | 1:M1:425:PHE:HA   | 2.16                     | 0.46              |
| 2:N1:62:ASN:HD21  | 2:N1:65:THR:CB    | 2.28                     | 0.46              |
| 2:N1:345:LYS:HG2  | 2:N1:418:VAL:CG1  | 2.46                     | 0.46              |
| 3:O1:373:GLU:O    | 3:O1:377:LEU:HD12 | 2.16                     | 0.46              |
| 4:P1:33:TYR:O     | 4:P1:37:CYS:N     | 2.41                     | 0.46              |
| 5:Q1:141:HIS:HB3  | 5:Q1:142:LEU:H    | 1.50                     | 0.46              |
| 17:82:186:ALA:HA  | 17:82:187:CYS:HA  | 1.57                     | 0.46              |
| 17:82:422:HIS:O   | 19:A2:76:ARG:HD2  | 2.16                     | 0.46              |
| 29:K2:31:GLN:HA   | 29:K2:34:ARG:HE   | 1.79                     | 0.46              |
| 37:T2:99:LEU:O    | 37:T2:103:ALA:N   | 2.47                     | 0.46              |
| 52:12:21:THR:CG2  | 52:12:25:ARG:NH2  | 2.79                     | 0.46              |
| 1:A1:192:ALA:HA   | 1:A1:194:ARG:N    | 2.31                     | 0.46              |
| 1:A1:389:ARG:C    | 1:A1:391:PRO:HD3  | 2.41                     | 0.46              |
| 2:B1:304:HIS:CD2  | 2:B1:305:GLN:N    | 2.84                     | 0.46              |
| 3:C1:6:LYS:HG2    | 3:C1:16:ASN:OD1   | 2.15                     | 0.46              |
| 3:C1:200:LEU:O    | 3:C1:200:LEU:HG   | 2.15                     | 0.46              |
| 3:C1:345:HIS:N    | 3:C1:346:PRO:HD2  | 2.29                     | 0.46              |
| 4:D1:23:HIS:O     | 4:D1:24:THR:C     | 2.55                     | 0.46              |
| 4:D1:98:PRO:O     | 4:D1:101:ALA:HB3  | 2.16                     | 0.46              |
| 4:D1:116:ILE:HD11 | 4:D1:120:ARG:HG3  | 1.97                     | 0.46              |
| 4:D1:150:ASN:OD1  | 4:D1:151:PRO:N    | 2.49                     | 0.46              |
| 6:F1:10:SER:HA    | 6:F1:13:LEU:CD1   | 2.45                     | 0.46              |
| 7:G1:50:PRO:CB    | 7:G1:51:PRO:CD    | 2.92                     | 0.46              |
| 1:M1:43:ALA:CB    | 1:M1:189:HIS:CB   | 2.94                     | 0.46              |
| 1:M1:75:LEU:HD12  | 1:M1:112:LEU:HD11 | 1.96                     | 0.46              |
| 2:N1:286:LYS:HZ2  | 2:N1:286:LYS:HG3  | 1.66                     | 0.46              |
| 3:O1:116:GLY:O    | 3:O1:119:LEU:HB2  | 2.16                     | 0.46              |
| 4:P1:138:PRO:CB   | 8:T1:55:THR:HA    | 2.46                     | 0.46              |
| 7:S1:73:ASN:N     | 7:S1:74:PRO:HD2   | 2.31                     | 0.46              |
| 19:A2:583:ILE:CD1 | 38:U2:137:TRP:CZ3 | 2.99                     | 0.46              |
| 20:B2:91:ALA:HB2  | 20:B2:193:ASP:CG  | 2.39                     | 0.46              |
| 20:B2:368:ARG:HA  | 20:B2:371:MET:HG2 | 1.98                     | 0.46              |
| 29:K2:15:GLY:HA2  | 29:K2:16:LEU:HA   | 1.58                     | 0.46              |
| 49:h2:111:ASP:OD1 | 49:h2:111:ASP:N   | 2.47                     | 0.46              |
| 56:A3:299:VAL:HA  | 56:A3:302:ARG:NH1 | 2.31                     | 0.46              |
| 65:J3:11:LEU:O    | 65:J3:11:LEU:HD23 | 2.15                     | 0.46              |
| 1:A1:39:VAL:CG1   | 1:A1:195:MET:CE   | 2.94                     | 0.45              |
| 1:A1:46:ARG:NH2   | 1:A1:316:ASP:CG   | 2.62                     | 0.45              |
| 1:A1:243:HIS:CD2  | 1:A1:425:PHE:CE2  | 3.04                     | 0.45              |
| 2:B1:264:ILE:HG21 | 2:B1:317:SER:HA   | 1.97                     | 0.45              |
| 3:C1:26:ASN:HA    | 6:F1:70:MET:HA    | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G1:48:VAL:O      | 7:G1:51:PRO:HD2    | 2.16                     | 0.45              |
| 10:J1:61:ASN:O     | 10:J1:62:LYS:HB2   | 2.15                     | 0.45              |
| 1:M1:40:TRP:HZ2    | 1:M1:377:GLU:CB    | 2.28                     | 0.45              |
| 1:M1:46:ARG:HB3    | 1:M1:92:ARG:O      | 2.15                     | 0.45              |
| 1:M1:130:GLU:O     | 1:M1:131:ARG:C     | 2.57                     | 0.45              |
| 1:M1:170:PRO:O     | 1:M1:171:SER:C     | 2.55                     | 0.45              |
| 1:M1:245:GLU:C     | 1:M1:247:GLY:H     | 2.24                     | 0.45              |
| 1:M1:252:HIS:O     | 1:M1:424:GLY:HA2   | 2.16                     | 0.45              |
| 1:M1:441:MET:HE3   | 1:M1:441:MET:HB3   | 1.74                     | 0.45              |
| 2:N1:352:LEU:HD21  | 2:N1:357:VAL:CG2   | 2.46                     | 0.45              |
| 3:O1:119:LEU:CD1   | 3:O1:192:ILE:HG22  | 2.45                     | 0.45              |
| 5:Q1:186:GLU:HG3   | 5:Q1:186:GLU:O     | 2.16                     | 0.45              |
| 10:V1:4:THR:O      | 10:V1:5:LEU:C      | 2.57                     | 0.45              |
| 12:22:113:PHE:HA   | 12:22:116:PRO:HD2  | 1.97                     | 0.45              |
| 16:72:140:ALA:HA   | 16:72:142:GLY:H    | 1.80                     | 0.45              |
| 19:A2:59:GLN:HB3   | 21:C2:241:TRP:HZ3  | 1.79                     | 0.45              |
| 19:A2:651:PRO:HD3  | 29:K2:22:HIS:CE1   | 2.50                     | 0.45              |
| 25:G2:97:TRP:HB2   | 25:G2:128:PHE:HB2  | 1.98                     | 0.45              |
| 26:H2:28:LYS:HB3   | 45:b2:184:LYS:HA   | 1.98                     | 0.45              |
| 27:I2:103:LEU:HD13 | 27:I2:121:GLN:HB3  | 1.98                     | 0.45              |
| 36:S2:196:ASP:HB3  | 36:S2:248:ALA:H    | 1.81                     | 0.45              |
| 37:T2:139:PRO:HB2  | 45:b2:161:ARG:HE   | 1.80                     | 0.45              |
| 46:c2:73:THR:HA    | 46:c2:77:ILE:HD12  | 1.97                     | 0.45              |
| 53:62:137:LEU:HB3  | 53:62:196:TRP:HD1  | 1.81                     | 0.45              |
| 57:B3:58:ALA:O     | 57:B3:60:GLU:HG3   | 2.16                     | 0.45              |
| 1:A1:349:ALA:O     | 1:A1:408:ARG:NH2   | 2.50                     | 0.45              |
| 2:B1:262:ALA:HB3   | 2:B1:269:ALA:N     | 2.31                     | 0.45              |
| 2:B1:395:PRO:O     | 2:B1:396:SER:C     | 2.59                     | 0.45              |
| 3:C1:152:ALA:N     | 3:C1:287:LYS:NZ    | 2.64                     | 0.45              |
| 5:E1:15:ARG:HH21   | 5:E1:32:ARG:CG     | 2.29                     | 0.45              |
| 10:J1:27:GLY:O     | 10:J1:28:ALA:C     | 2.59                     | 0.45              |
| 10:J1:57:HIS:O     | 10:J1:60:GLU:HG2   | 2.17                     | 0.45              |
| 1:M1:53:ASN:CG     | 1:M1:170:PRO:HD3   | 2.41                     | 0.45              |
| 1:M1:64:PHE:CZ     | 1:M1:88:ALA:HB2    | 2.51                     | 0.45              |
| 1:M1:262:TRP:CD2   | 1:M1:385:THR:CG2   | 2.97                     | 0.45              |
| 1:M1:262:TRP:CE3   | 1:M1:385:THR:HG23  | 2.52                     | 0.45              |
| 1:M1:408:ARG:HH12  | 11:W1:15:ARG:CD    | 2.28                     | 0.45              |
| 4:P1:50:HIS:O      | 4:P1:54:VAL:N      | 2.32                     | 0.45              |
| 4:P1:227:TRP:CE3   | 4:P1:230:LEU:HD12  | 2.51                     | 0.45              |
| 14:42:318:ALA:HB1  | 14:42:374:ASN:HD22 | 1.82                     | 0.45              |
| 17:82:415:ILE:HG23 | 19:A2:119:PHE:HZ   | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:92:164:THR:HB   | 18:92:169:PHE:HB2  | 1.98                     | 0.45              |
| 19:A2:153:PHE:HE2  | 19:A2:156:GLY:HA3  | 1.81                     | 0.45              |
| 19:A2:613:PRO:HB2  | 38:U2:134:ILE:HG21 | 1.91                     | 0.45              |
| 23:E2:158:CYS:SG   | 23:E2:159:GLN:N    | 2.89                     | 0.45              |
| 27:I2:111:THR:HG22 | 27:I2:118:GLN:HA   | 1.97                     | 0.45              |
| 38:U2:42:ASP:HA    | 38:U2:43:LYS:HA    | 1.75                     | 0.45              |
| 56:A3:32:ALA:HB3   | 67:L3:36:PRO:HG2   | 1.98                     | 0.45              |
| 56:A3:147:ILE:HD11 | 56:A3:209:LEU:HD23 | 1.98                     | 0.45              |
| 56:A3:172:LYS:HB2  | 56:A3:172:LYS:HZ3  | 1.81                     | 0.45              |
| 56:A3:435:GLY:O    | 56:A3:437:PRO:HD3  | 2.15                     | 0.45              |
| 1:A1:179:ARG:HG3   | 1:A1:180:ALA:N     | 2.31                     | 0.45              |
| 2:B1:71:LEU:HD13   | 2:B1:143:GLN:HG3   | 1.97                     | 0.45              |
| 2:B1:338:LYS:HD3   | 2:B1:439:LEU:CD2   | 2.46                     | 0.45              |
| 3:C1:61:THR:O      | 3:C1:64:SER:HB3    | 2.16                     | 0.45              |
| 3:C1:136:GLY:O     | 3:C1:139:SER:N     | 2.49                     | 0.45              |
| 4:D1:180:SER:HB3   | 8:H1:17:LEU:HB2    | 1.98                     | 0.45              |
| 7:G1:11:ARG:HB3    | 7:G1:12:HIS:CD2    | 2.50                     | 0.45              |
| 10:J1:55:ILE:CG2   | 10:J1:58:LYS:HE2   | 2.44                     | 0.45              |
| 2:N1:35:ILE:HD11   | 2:N1:213:HIS:CD2   | 2.50                     | 0.45              |
| 3:O1:352:GLN:O     | 3:O1:356:VAL:HG23  | 2.17                     | 0.45              |
| 4:P1:26:ILE:HG21   | 4:P1:54:VAL:HG22   | 1.98                     | 0.45              |
| 4:P1:178:THR:HB    | 4:P1:181:GLN:CG    | 2.32                     | 0.45              |
| 8:T1:40:CYS:O      | 8:T1:44:VAL:HG23   | 2.15                     | 0.45              |
| 8:T1:65:ARG:O      | 8:T1:69:VAL:HG23   | 2.16                     | 0.45              |
| 10:V1:55:ILE:CG2   | 10:V1:58:LYS:HE2   | 2.45                     | 0.45              |
| 14:42:393:ILE:HG21 | 53:62:184:LEU:HD13 | 1.98                     | 0.45              |
| 17:82:415:ILE:HD12 | 19:A2:119:PHE:CE1  | 2.51                     | 0.45              |
| 19:A2:181:ARG:N    | 75:A2:802:SF4:S2   | 2.89                     | 0.45              |
| 19:A2:306:MET:HA   | 19:A2:316:HIS:HA   | 1.98                     | 0.45              |
| 19:A2:381:LEU:HD12 | 29:K2:55:ILE:HG21  | 1.99                     | 0.45              |
| 34:Q2:111:VAL:O    | 34:Q2:117:TRP:N    | 2.44                     | 0.45              |
| 36:S2:114:GLY:HA3  | 36:S2:115:ASN:HA   | 1.62                     | 0.45              |
| 57:B3:76:ILE:O     | 57:B3:79:PRO:HD2   | 2.16                     | 0.45              |
| 1:A1:255:ILE:HD12  | 1:A1:335:MET:CE    | 2.47                     | 0.45              |
| 1:A1:394:GLU:O     | 1:A1:397:SER:OG    | 2.26                     | 0.45              |
| 2:B1:46:ARG:NH1    | 2:B1:376:GLU:HG3   | 2.30                     | 0.45              |
| 2:B1:83:PHE:CZ     | 6:R1:104:ARG:HG2   | 2.52                     | 0.45              |
| 2:B1:161:GLU:CD    | 2:B1:175:SER:HB2   | 2.40                     | 0.45              |
| 2:B1:201:SER:HG    | 2:B1:226:ILE:H     | 1.61                     | 0.45              |
| 2:B1:243:GLU:HA    | 2:B1:424:MET:O     | 2.17                     | 0.45              |
| 2:B1:267:ALA:O     | 2:B1:268:GLU:C     | 2.59                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B1:270:ASN:O    | 2:B1:271:ALA:C     | 2.59                     | 0.45              |
| 2:B1:360:ALA:O    | 2:B1:361:LYS:C     | 2.60                     | 0.45              |
| 3:C1:26:ASN:HD22  | 3:C1:208:PRO:HD2   | 1.82                     | 0.45              |
| 3:C1:90:PHE:CE1   | 3:C1:123:VAL:HG11  | 2.51                     | 0.45              |
| 3:C1:136:GLY:O    | 3:C1:138:MET:N     | 2.49                     | 0.45              |
| 3:C1:149:LEU:O    | 3:C1:291:VAL:HG21  | 2.15                     | 0.45              |
| 4:D1:23:HIS:CD2   | 10:J1:50:LYS:O     | 2.70                     | 0.45              |
| 4:D1:35:GLN:HB2   | 4:D1:169:LEU:HD11  | 1.98                     | 0.45              |
| 4:D1:74:PRO:CG    | 4:D1:82:MET:HB3    | 2.46                     | 0.45              |
| 10:J1:52:TRP:N    | 10:J1:52:TRP:HE3   | 2.14                     | 0.45              |
| 1:M1:125:SER:O    | 1:M1:129:LYS:HG3   | 2.16                     | 0.45              |
| 1:M1:294:LEU:HD23 | 1:M1:337:VAL:HG12  | 1.98                     | 0.45              |
| 1:M1:430:GLN:CG   | 1:M1:430:GLN:O     | 2.63                     | 0.45              |
| 3:O1:10:LEU:O     | 3:O1:13:ILE:HG13   | 2.17                     | 0.45              |
| 3:O1:24:PRO:O     | 3:O1:224:TYR:OH    | 2.22                     | 0.45              |
| 3:O1:26:ASN:HB2   | 6:R1:69:SER:OG     | 2.17                     | 0.45              |
| 3:O1:63:PHE:O     | 3:O1:67:THR:OG1    | 2.33                     | 0.45              |
| 3:O1:115:ILE:HG22 | 3:O1:196:HIS:HB2   | 1.97                     | 0.45              |
| 4:P1:228:SER:HB2  | 7:S1:23:GLN:NE2    | 2.32                     | 0.45              |
| 5:Q1:138:VAL:O    | 5:Q1:139:CYS:C     | 2.59                     | 0.45              |
| 6:R1:7:SER:O      | 6:R1:11:ARG:HB2    | 2.16                     | 0.45              |
| 20:B2:97:LEU:HB3  | 20:B2:111:PRO:HA   | 1.98                     | 0.45              |
| 45:b2:70:LEU:HA   | 45:b2:73:PHE:HB3   | 1.97                     | 0.45              |
| 53:62:352:ASP:OD1 | 53:62:352:ASP:N    | 2.49                     | 0.45              |
| 56:A3:158:ILE:O   | 56:A3:162:ILE:HG13 | 2.17                     | 0.45              |
| 56:A3:240:HIS:O   | 56:A3:243:VAL:HG22 | 2.16                     | 0.45              |
| 56:A3:273:MET:HG3 | 56:A3:319:LYS:NZ   | 2.31                     | 0.45              |
| 1:A1:195:MET:HE2  | 1:A1:195:MET:HB3   | 1.82                     | 0.45              |
| 2:B1:213:HIS:H    | 2:B1:214:PRO:HD2   | 1.77                     | 0.45              |
| 3:C1:148:ASN:O    | 3:C1:151:SER:OG    | 2.26                     | 0.45              |
| 4:D1:35:GLN:HA    | 4:D1:35:GLN:OE1    | 2.16                     | 0.45              |
| 4:D1:168:VAL:HG12 | 4:D1:169:LEU:CD2   | 2.47                     | 0.45              |
| 7:G1:71:ARG:O     | 7:G1:73:ASN:N      | 2.50                     | 0.45              |
| 1:M1:246:ASP:HA   | 1:M1:427:PRO:HD3   | 1.97                     | 0.45              |
| 2:N1:109:VAL:HG22 | 2:N1:119:LEU:HD23  | 1.99                     | 0.45              |
| 2:N1:141:GLN:CB   | 2:N1:142:PRO:HD3   | 2.46                     | 0.45              |
| 2:N1:159:VAL:CG1  | 2:N1:160:ILE:N     | 2.79                     | 0.45              |
| 2:N1:235:ALA:O    | 2:N1:236:LYS:CB    | 2.65                     | 0.45              |
| 2:N1:258:VAL:HG21 | 2:N1:312:PHE:HD2   | 1.82                     | 0.45              |
| 2:N1:396:SER:O    | 2:N1:399:LEU:HB2   | 2.15                     | 0.45              |
| 3:O1:28:SER:CB    | 3:O1:30:TRP:HD1    | 2.26                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O1:309:THR:HG23 | 3:O1:310:SER:N    | 2.30                     | 0.45              |
| 3:O1:338:ILE:HA   | 3:O1:341:GLN:HG3  | 1.99                     | 0.45              |
| 6:R1:48:ARG:HD3   | 6:R1:48:ARG:HA    | 1.51                     | 0.45              |
| 6:R1:64:ARG:O     | 6:R1:68:LEU:HD12  | 2.16                     | 0.45              |
| 6:R1:70:MET:HE3   | 6:R1:70:MET:HB3   | 1.65                     | 0.45              |
| 12:22:258:SER:HA  | 12:22:334:THR:HB  | 1.99                     | 0.45              |
| 22:D2:113:PHE:HB2 | 22:D2:114:ARG:NE  | 2.28                     | 0.45              |
| 46:c2:20:ARG:O    | 46:c2:24:LYS:N    | 2.41                     | 0.45              |
| 61:F3:40:SER:OG   | 61:F3:45:ASP:HB3  | 2.16                     | 0.45              |
| 1:A1:332:ASP:O    | 1:A1:332:ASP:OD1  | 2.34                     | 0.45              |
| 1:A1:341:GLN:OE1  | 1:A1:344:ARG:HD3  | 2.16                     | 0.45              |
| 4:D1:80:MET:H     | 4:D1:80:MET:HG2   | 1.47                     | 0.45              |
| 4:D1:165:TYR:CD2  | 4:D1:168:VAL:HG22 | 2.52                     | 0.45              |
| 1:M1:16:VAL:HG11  | 1:M1:388:ARG:HB2  | 1.98                     | 0.45              |
| 1:M1:43:ALA:HB2   | 1:M1:189:HIS:HB3  | 1.99                     | 0.45              |
| 1:M1:241:ILE:HG21 | 1:M1:241:ILE:HD13 | 1.64                     | 0.45              |
| 1:M1:329:MET:HG3  | 7:S1:2:ARG:HH11   | 1.82                     | 0.45              |
| 1:M1:333:ASP:O    | 1:M1:334:MET:C    | 2.58                     | 0.45              |
| 2:N1:53:ALA:HB2   | 2:N1:198:HIS:HB3  | 1.99                     | 0.45              |
| 3:O1:44:GLN:OE1   | 3:O1:83:HIS:CE1   | 2.69                     | 0.45              |
| 3:O1:218:ILE:CG2  | 3:O1:219:PRO:HD2  | 2.46                     | 0.45              |
| 3:O1:347:TYR:O    | 3:O1:348:ILE:C    | 2.58                     | 0.45              |
| 4:P1:161:ALA:O    | 4:P1:163:PRO:N    | 2.49                     | 0.45              |
| 4:P1:220:TYR:CD2  | 7:S1:26:PHE:CZ    | 3.04                     | 0.45              |
| 7:S1:44:CYS:O     | 7:S1:45:ILE:C     | 2.59                     | 0.45              |
| 11:W1:24:TRP:O    | 11:W1:25:GLY:C    | 2.59                     | 0.45              |
| 14:42:307:TRP:HE1 | 53:62:71:ILE:HD12 | 1.81                     | 0.45              |
| 17:82:177:TYR:HD1 | 17:82:182:ILE:HB  | 1.82                     | 0.45              |
| 18:92:42:ARG:HH12 | 19:A2:199:GLY:C   | 2.25                     | 0.45              |
| 19:A2:557:ARG:CZ  | 38:U2:144:TYR:CZ  | 2.98                     | 0.45              |
| 35:R2:52:SER:OG   | 35:R2:77:GLY:O    | 2.26                     | 0.45              |
| 35:R2:155:VAL:O   | 35:R2:159:ALA:N   | 2.49                     | 0.45              |
| 57:B3:78:LEU:HB2  | 57:B3:79:PRO:CD   | 2.38                     | 0.45              |
| 1:A1:64:PHE:CZ    | 1:A1:88:ALA:HB2   | 2.51                     | 0.45              |
| 1:A1:444:LEU:HA   | 1:A1:444:LEU:HD12 | 1.82                     | 0.45              |
| 2:B1:56:ARG:HH21  | 2:B1:103:GLU:CD   | 2.25                     | 0.45              |
| 4:D1:28:ARG:HB2   | 4:D1:185:ASP:HB3  | 1.99                     | 0.45              |
| 4:D1:221:ALA:O    | 4:D1:222:MET:C    | 2.57                     | 0.45              |
| 6:F1:43:VAL:O     | 6:F1:44:LYS:C     | 2.57                     | 0.45              |
| 6:F1:67:ASP:HA    | 6:F1:70:MET:HE2   | 1.98                     | 0.45              |
| 1:M1:426:GLY:H    | 1:M1:428:ILE:HD11 | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N1:239:TYR:HE2   | 2:N1:421:ARG:HB3   | 1.81                     | 0.45              |
| 2:N1:261:SER:HB3   | 2:N1:321:LEU:C     | 2.42                     | 0.45              |
| 2:N1:308:ASP:O     | 2:N1:309:VAL:HG23  | 2.17                     | 0.45              |
| 2:N1:314:ALA:HB1   | 9:U1:64:LEU:HD22   | 1.97                     | 0.45              |
| 2:N1:338:LYS:O     | 2:N1:341:TYR:N     | 2.50                     | 0.45              |
| 3:O1:183:PHE:CD1   | 3:O1:183:PHE:C     | 2.94                     | 0.45              |
| 4:P1:23:HIS:CD2    | 10:V1:52:TRP:N     | 2.85                     | 0.45              |
| 5:Q1:120:PRO:O     | 5:Q1:121:GLN:NE2   | 2.49                     | 0.45              |
| 10:V1:52:TRP:CG    | 10:V1:53:LYS:N     | 2.84                     | 0.45              |
| 13:32:60:ILE:HG21  | 16:72:168:ILE:HG21 | 1.97                     | 0.45              |
| 14:42:115:LEU:HD12 | 14:42:174:LEU:HB2  | 1.98                     | 0.45              |
| 14:42:207:MET:HA   | 14:42:208:PRO:HD3  | 1.82                     | 0.45              |
| 17:82:318:ILE:HD13 | 17:82:355:ILE:HG13 | 1.99                     | 0.45              |
| 19:A2:381:LEU:HD11 | 19:A2:664:TYR:HD2  | 1.81                     | 0.45              |
| 34:Q2:121:ASP:N    | 34:Q2:121:ASP:OD1  | 2.49                     | 0.45              |
| 43:Z2:44:PRO:HA    | 43:Z2:45:TRP:HA    | 1.81                     | 0.45              |
| 60:E3:78:HIS:CE1   | 64:I3:12:LEU:HD22  | 2.52                     | 0.45              |
| 1:A1:39:VAL:HG22   | 1:A1:197:LEU:HD22  | 1.98                     | 0.45              |
| 1:A1:197:LEU:HD11  | 1:A1:208:LEU:HD11  | 1.98                     | 0.45              |
| 1:A1:255:ILE:HG13  | 1:A1:422:VAL:HG22  | 1.98                     | 0.45              |
| 1:A1:392:LEU:HA    | 1:A1:395:TRP:NE1   | 2.30                     | 0.45              |
| 2:B1:160:ILE:HD13  | 2:B1:160:ILE:N     | 2.31                     | 0.45              |
| 2:B1:262:ALA:HB2   | 2:B1:268:GLU:HB3   | 1.98                     | 0.45              |
| 3:C1:25:SER:HA     | 3:C1:218:ILE:HD11  | 1.98                     | 0.45              |
| 3:C1:47:THR:HG23   | 3:C1:79:ILE:HG23   | 1.99                     | 0.45              |
| 3:C1:182:HIS:O     | 3:C1:186:PRO:CD    | 2.64                     | 0.45              |
| 4:D1:32:VAL:HG11   | 4:D1:186:VAL:HG22  | 1.97                     | 0.45              |
| 5:E1:45:VAL:HG13   | 10:J1:28:ALA:CA    | 2.46                     | 0.45              |
| 1:M1:50:GLU:O      | 1:M1:173:ASN:ND2   | 2.49                     | 0.45              |
| 1:M1:394:GLU:O     | 1:M1:397:SER:N     | 2.49                     | 0.45              |
| 1:M1:444:LEU:HD12  | 1:M1:444:LEU:HA    | 1.73                     | 0.45              |
| 2:N1:50:PHE:CE1    | 2:N1:207:ILE:HG13  | 2.52                     | 0.45              |
| 2:N1:182:ARG:O     | 2:N1:185:LYS:HB3   | 2.17                     | 0.45              |
| 3:O1:147:THR:CG2   | 3:O1:165:TRP:NE1   | 2.75                     | 0.45              |
| 3:O1:316:MET:HE2   | 3:O1:317:PHE:CZ    | 2.51                     | 0.45              |
| 5:Q1:7:VAL:HG13    | 5:Q1:8:PRO:HD2     | 1.98                     | 0.45              |
| 5:Q1:131:GLU:HG2   | 5:Q1:132:TRP:CD1   | 2.51                     | 0.45              |
| 10:V1:23:THR:O     | 10:V1:24:ILE:C     | 2.58                     | 0.45              |
| 72:22:401:3PE:H292 | 72:22:401:3PE:H2E1 | 1.98                     | 0.45              |
| 19:A2:81:GLU:HG3   | 19:A2:108:LYS:HD2  | 1.99                     | 0.45              |
| 35:R2:275:ASP:O    | 35:R2:279:TYR:N    | 2.48                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:62:307:SER:HA   | 53:62:310:LEU:HD12 | 1.99                     | 0.45              |
| 57:B3:41:ILE:O     | 57:B3:45:MET:HG2   | 2.16                     | 0.45              |
| 57:B3:98:LYS:HB2   | 57:B3:98:LYS:HE3   | 1.79                     | 0.45              |
| 67:L3:35:ALA:HB3   | 67:L3:36:PRO:HD3   | 1.99                     | 0.45              |
| 1:A1:46:ARG:NH1    | 1:A1:316:ASP:OD1   | 2.50                     | 0.45              |
| 1:A1:106:LEU:N     | 1:A1:107:PRO:CD    | 2.77                     | 0.45              |
| 1:A1:236:PHE:HD2   | 1:A1:258:GLU:CB    | 2.28                     | 0.45              |
| 1:A1:240:GLN:HE21  | 1:A1:431:LEU:HD21  | 1.81                     | 0.45              |
| 1:A1:345:LEU:HD23  | 1:A1:345:LEU:HA    | 1.68                     | 0.45              |
| 2:B1:271:ALA:O     | 2:B1:272:PHE:C     | 2.58                     | 0.45              |
| 3:C1:53:MET:SD     | 3:O1:181:PHE:CZ    | 3.10                     | 0.45              |
| 5:E1:7:VAL:HG13    | 7:G1:16:TYR:CD1    | 2.51                     | 0.45              |
| 1:M1:76:GLU:O      | 1:M1:77:LYS:C      | 2.60                     | 0.45              |
| 1:M1:272:VAL:HG13  | 1:M1:358:LYS:HA    | 1.98                     | 0.45              |
| 2:N1:135:TRP:CD1   | 2:N1:136:GLU:HG3   | 2.52                     | 0.45              |
| 2:N1:159:VAL:CG1   | 2:N1:160:ILE:HD13  | 2.40                     | 0.45              |
| 2:N1:203:ARG:NH2   | 2:N1:230:LEU:HD23  | 2.31                     | 0.45              |
| 3:O1:337:TRP:O     | 3:O1:341:GLN:HG2   | 2.17                     | 0.45              |
| 4:P1:102:ARG:O     | 4:P1:106:ASN:N     | 2.49                     | 0.45              |
| 7:S1:34:ILE:CB     | 7:S1:35:PRO:CD     | 2.91                     | 0.45              |
| 9:U1:64:LEU:CG     | 9:U1:65:VAL:HG23   | 2.41                     | 0.45              |
| 19:A2:181:ARG:CB   | 75:A2:802:SF4:S2   | 3.03                     | 0.45              |
| 72:B2:501:3PE:H382 | 52:12:180:PRO:HB3  | 1.99                     | 0.45              |
| 53:62:161:ARG:NH2  | 53:62:238:GLU:OE1  | 2.49                     | 0.45              |
| 54:g2:4:SER:OG     | 54:g2:5:TRP:N      | 2.45                     | 0.45              |
| 54:g2:146:LEU:HA   | 54:g2:147:GLY:HA2  | 1.67                     | 0.45              |
| 56:A3:431:LEU:HD21 | 56:A3:450:TRP:HB2  | 1.99                     | 0.45              |
| 79:A3:602:HEA:HHC  | 79:A3:602:HEA:O11  | 2.17                     | 0.45              |
| 58:C3:42:LEU:HD12  | 58:C3:42:LEU:HA    | 1.66                     | 0.45              |
| 62:G3:3:ALA:O      | 62:G3:4:ALA:HB2    | 2.17                     | 0.45              |
| 65:J3:2:GLU:CG     | 65:J3:3:ASN:H      | 2.30                     | 0.45              |
| 1:A1:17:SER:HB2    | 1:A1:25:VAL:HB     | 1.99                     | 0.45              |
| 1:A1:184:GLU:O     | 1:A1:185:TYR:C     | 2.59                     | 0.45              |
| 2:B1:29:LEU:HD12   | 2:B1:33:LEU:HD21   | 1.98                     | 0.45              |
| 2:B1:42:ALA:HB1    | 2:B1:43:PRO:CD     | 2.40                     | 0.45              |
| 2:B1:124:LEU:HD13  | 2:B1:223:PHE:CG    | 2.52                     | 0.45              |
| 3:C1:125:ALA:HB3   | 3:C1:185:LEU:HD21  | 1.98                     | 0.45              |
| 3:C1:153:ILE:HD12  | 3:C1:153:ILE:H     | 1.82                     | 0.45              |
| 4:D1:228:SER:HB2   | 7:G1:23:GLN:HE21   | 1.74                     | 0.45              |
| 7:G1:75:ALA:O      | 7:G1:76:ALA:C      | 2.60                     | 0.45              |
| 1:M1:233:PRO:HG2   | 5:Q1:23:LYS:HD3    | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:339:GLN:O     | 1:M1:343:MET:HG2   | 2.17                     | 0.45              |
| 1:M1:426:GLY:CA    | 1:M1:427:PRO:C     | 2.90                     | 0.45              |
| 2:N1:300:ALA:HA    | 2:N1:307:PHE:HZ    | 1.77                     | 0.45              |
| 3:O1:137:GLN:HE22  | 3:O1:263:ASN:HB3   | 1.80                     | 0.45              |
| 4:P1:143:LEU:HD11  | 4:P1:149:PHE:HB2   | 1.98                     | 0.45              |
| 17:82:413:TRP:HE1  | 17:82:436:GLN:HG3  | 1.82                     | 0.45              |
| 18:92:110:MET:CG   | 19:A2:194:ASP:C    | 2.88                     | 0.45              |
| 23:E2:115:ALA:O    | 23:E2:140:ARG:NH1  | 2.40                     | 0.45              |
| 53:62:171:ALA:O    | 53:62:175:ASN:ND2  | 2.50                     | 0.45              |
| 61:F3:31:TYR:HE1   | 61:F3:98:HIS:CE1   | 2.34                     | 0.45              |
| 2:B1:299:VAL:CG1   | 2:B1:303:VAL:HG21  | 2.46                     | 0.44              |
| 2:B1:346:THR:O     | 2:B1:349:GLN:N     | 2.39                     | 0.44              |
| 3:C1:113:TRP:O     | 3:C1:117:VAL:HG23  | 2.17                     | 0.44              |
| 3:C1:177:ARG:HG2   | 3:C1:181:PHE:HE2   | 1.82                     | 0.44              |
| 3:C1:183:PHE:HZ    | 3:O1:184:ILE:HB    | 1.82                     | 0.44              |
| 4:D1:25:SER:O      | 4:D1:26:ILE:C      | 2.58                     | 0.44              |
| 4:D1:197:GLU:O     | 4:D1:198:HIS:C     | 2.59                     | 0.44              |
| 1:M1:430:GLN:O     | 1:M1:430:GLN:HG2   | 2.16                     | 0.44              |
| 2:N1:54:GLY:H      | 2:N1:57:TYR:HD1    | 1.65                     | 0.44              |
| 3:O1:55:TYR:CE2    | 3:O1:56:THR:O      | 2.70                     | 0.44              |
| 3:O1:90:PHE:CE1    | 3:O1:123:VAL:HG11  | 2.52                     | 0.44              |
| 3:O1:107:TYR:OH    | 3:O1:308:HIS:HB2   | 2.17                     | 0.44              |
| 3:O1:185:LEU:N     | 3:O1:186:PRO:CD    | 2.80                     | 0.44              |
| 3:O1:277:ALA:HB1   | 3:O1:294:LEU:HD11  | 1.99                     | 0.44              |
| 3:O1:341:GLN:HA    | 3:O1:341:GLN:HE21  | 1.82                     | 0.44              |
| 4:P1:55:CYS:SG     | 10:V1:52:TRP:HA    | 2.57                     | 0.44              |
| 4:P1:65:ALA:O      | 4:P1:69:GLU:OE2    | 2.35                     | 0.44              |
| 4:P1:136:GLU:O     | 4:P1:137:PRO:C     | 2.60                     | 0.44              |
| 20:B2:382:PHE:HD1  | 23:E2:118:LEU:HD11 | 1.81                     | 0.44              |
| 21:C2:117:THR:OG1  | 21:C2:118:ALA:N    | 2.50                     | 0.44              |
| 22:D2:150:VAL:HG12 | 22:D2:179:VAL:HG13 | 1.99                     | 0.44              |
| 35:R2:64:PHE:HZ    | 35:R2:208:GLY:HA3  | 1.82                     | 0.44              |
| 36:S2:338:LYS:HZ3  | 51:j2:51:ARG:HH11  | 1.64                     | 0.44              |
| 39:V2:28:ARG:HA    | 39:V2:29:GLY:HA3   | 1.70                     | 0.44              |
| 44:a2:104:VAL:O    | 44:a2:107:THR:OG1  | 2.31                     | 0.44              |
| 51:j2:83:TYR:HD1   | 51:j2:86:ARG:HH21  | 1.65                     | 0.44              |
| 56:A3:379:TYR:CE2  | 56:A3:383:MET:HE2  | 2.52                     | 0.44              |
| 57:B3:121:TYR:C    | 57:B3:138:VAL:HG23 | 2.42                     | 0.44              |
| 58:C3:183:GLU:O    | 62:G3:42:ARG:NH2   | 2.50                     | 0.44              |
| 2:B1:211:VAL:CG1   | 2:B1:212:SER:N     | 2.81                     | 0.44              |
| 3:C1:183:PHE:CE1   | 3:C1:187:PHE:HE2   | 2.35                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C1:315:MET:O    | 3:C1:318:ARG:N     | 2.35                     | 0.44              |
| 3:C1:371:THR:O    | 3:C1:372:ILE:C     | 2.61                     | 0.44              |
| 4:D1:31:GLN:OE1   | 4:D1:31:GLN:HA     | 2.17                     | 0.44              |
| 4:D1:67:GLU:O     | 4:D1:70:VAL:HG12   | 2.17                     | 0.44              |
| 6:F1:58:ARG:HG2   | 6:F1:58:ARG:HH11   | 1.82                     | 0.44              |
| 9:I1:51:CYS:SG    | 9:I1:53:GLU:HB3    | 2.57                     | 0.44              |
| 10:J1:4:THR:HG22  | 10:J1:6:THR:N      | 2.33                     | 0.44              |
| 1:M1:37:VAL:HG13  | 1:M1:199:ALA:CB    | 2.45                     | 0.44              |
| 2:N1:198:HIS:HE1  | 2:N1:233:SER:HB3   | 1.81                     | 0.44              |
| 3:O1:48:GLY:HA3   | 69:O1:401:HEM:C3C  | 2.52                     | 0.44              |
| 3:O1:264:THR:O    | 3:O1:266:PRO:HD3   | 2.16                     | 0.44              |
| 3:O1:364:VAL:O    | 3:O1:367:PRO:HG2   | 2.17                     | 0.44              |
| 4:P1:116:ILE:HD12 | 4:P1:116:ILE:HA    | 1.74                     | 0.44              |
| 5:Q1:171:ILE:O    | 5:Q1:171:ILE:CG2   | 2.62                     | 0.44              |
| 9:U1:57:GLY:O     | 9:U1:78:TYR:CE2    | 2.70                     | 0.44              |
| 19:A2:275:PRO:HB3 | 19:A2:286:ILE:HB   | 1.99                     | 0.44              |
| 23:E2:196:LYS:HD2 | 23:E2:197:TRP:CZ3  | 2.52                     | 0.44              |
| 36:S2:175:TYR:O   | 36:S2:179:LYS:N    | 2.45                     | 0.44              |
| 53:G2:199:GLN:O   | 54:G2:114:GLN:NE2  | 2.40                     | 0.44              |
| 56:A3:131:PRO:HB2 | 57:B3:159:VAL:HA   | 2.00                     | 0.44              |
| 57:B3:1:MET:SD    | 57:B3:133:LEU:HD13 | 2.58                     | 0.44              |
| 1:A1:197:LEU:CD1  | 1:A1:208:LEU:HD11  | 2.47                     | 0.44              |
| 1:A1:252:HIS:NE2  | 1:A1:325:VAL:HG21  | 2.32                     | 0.44              |
| 2:B1:314:ALA:CB   | 9:I1:64:LEU:HD22   | 2.48                     | 0.44              |
| 3:C1:26:ASN:CA    | 6:F1:70:MET:HB2    | 2.48                     | 0.44              |
| 3:C1:271:GLU:OE2  | 3:C1:273:TYR:OH    | 2.35                     | 0.44              |
| 3:C1:281:LEU:HD12 | 3:C1:281:LEU:O     | 2.16                     | 0.44              |
| 4:D1:167:GLU:HG2  | 4:D1:167:GLU:O     | 2.17                     | 0.44              |
| 4:D1:175:THR:HA   | 4:D1:176:PRO:HD2   | 1.73                     | 0.44              |
| 4:D1:229:VAL:HG12 | 4:D1:229:VAL:O     | 2.18                     | 0.44              |
| 1:M1:82:MET:HE2   | 1:M1:82:MET:HB2    | 1.93                     | 0.44              |
| 1:M1:157:ALA:HB2  | 1:M1:421:ALA:HB1   | 2.00                     | 0.44              |
| 2:N1:81:SER:O     | 2:N1:84:LYS:N      | 2.50                     | 0.44              |
| 2:N1:275:LEU:O    | 2:N1:276:GLN:C     | 2.60                     | 0.44              |
| 5:Q1:40:THR:CG2   | 10:V1:20:PHE:HZ    | 2.28                     | 0.44              |
| 5:Q1:134:ILE:C    | 5:Q1:135:LEU:HD23  | 2.42                     | 0.44              |
| 6:R1:43:VAL:HG22  | 6:R1:94:LEU:CD2    | 2.46                     | 0.44              |
| 10:V1:49:GLY:HA2  | 10:V1:54:HIS:HB3   | 1.98                     | 0.44              |
| 11:W1:23:LEU:N    | 11:W1:23:LEU:HD23  | 2.32                     | 0.44              |
| 14:42:370:PRO:HA  | 14:42:375:LEU:HB2  | 1.99                     | 0.44              |
| 17:82:146:GLY:O   | 17:82:150:GLY:N    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:82:246:GLU:HA  | 17:82:249:ALA:HB3  | 1.98                     | 0.44              |
| 19:A2:388:ASN:ND2 | 19:A2:513:MET:O    | 2.36                     | 0.44              |
| 30:L2:56:PRO:HG3  | 34:Q2:41:LYS:HB3   | 2.00                     | 0.44              |
| 31:N2:56:LEU:HA   | 31:N2:59:VAL:HB    | 1.99                     | 0.44              |
| 42:Y2:66:ALA:O    | 42:Y2:70:PHE:N     | 2.50                     | 0.44              |
| 52:12:3:MET:HA    | 52:12:6:ILE:HD12   | 2.00                     | 0.44              |
| 56:A3:51:ASP:O    | 56:A3:55:ASN:HB2   | 2.17                     | 0.44              |
| 57:B3:122:MET:HB2 | 57:B3:208:PRO:CD   | 2.47                     | 0.44              |
| 59:D3:79:LYS:NZ   | 66:K3:15:ASN:HD21  | 2.15                     | 0.44              |
| 64:I3:21:ILE:HD12 | 64:I3:21:ILE:HA    | 1.82                     | 0.44              |
| 1:A1:152:TYR:OH   | 1:A1:243:HIS:CD2   | 2.70                     | 0.44              |
| 2:B1:112:LEU:HD22 | 2:B1:112:LEU:HA    | 1.79                     | 0.44              |
| 3:C1:243:VAL:O    | 3:C1:243:VAL:HG22  | 2.17                     | 0.44              |
| 3:C1:310:SER:OG   | 3:C1:312:GLN:N     | 2.48                     | 0.44              |
| 4:D1:5:LEU:HG     | 4:D1:152:TYR:CE1   | 2.51                     | 0.44              |
| 5:E1:15:ARG:H     | 5:E1:15:ARG:HG2    | 1.66                     | 0.44              |
| 10:J1:18:SER:CB   | 11:K1:23:LEU:HD12  | 2.30                     | 0.44              |
| 2:N1:51:ILE:HD13  | 2:N1:199:PHE:CD2   | 2.53                     | 0.44              |
| 2:N1:322:PHE:CD1  | 2:N1:322:PHE:C     | 2.96                     | 0.44              |
| 2:N1:380:ASP:O    | 2:N1:381:GLU:C     | 2.61                     | 0.44              |
| 4:P1:165:TYR:CZ   | 4:P1:168:VAL:HG22  | 2.53                     | 0.44              |
| 4:P1:218:LEU:HD23 | 4:P1:218:LEU:HA    | 1.73                     | 0.44              |
| 6:R1:28:LYS:HB3   | 6:R1:74:ILE:CD1    | 2.47                     | 0.44              |
| 6:R1:37:ILE:CG1   | 6:R1:43:VAL:HG21   | 2.40                     | 0.44              |
| 12:22:173:THR:O   | 12:22:226:THR:OG1  | 2.27                     | 0.44              |
| 19:A2:215:MET:SD  | 19:A2:695:TYR:OH   | 2.73                     | 0.44              |
| 20:B2:293:LEU:HB3 | 20:B2:294:ARG:H    | 1.51                     | 0.44              |
| 20:B2:359:ASP:HB2 | 33:P2:45:PRO:HG2   | 2.00                     | 0.44              |
| 56:A3:195:LEU:CD2 | 56:A3:245:ILE:HD13 | 2.45                     | 0.44              |
| 56:A3:449:MET:HE3 | 66:K3:40:TRP:HB3   | 1.98                     | 0.44              |
| 57:B3:60:GLU:CD   | 57:B3:61:VAL:H     | 2.25                     | 0.44              |
| 61:F3:33:ILE:HG22 | 61:F3:34:LEU:HD12  | 1.98                     | 0.44              |
| 1:A1:199:ALA:HB3  | 1:A1:208:LEU:HD21  | 1.99                     | 0.44              |
| 1:A1:349:ALA:HB3  | 1:A1:408:ARG:CG    | 2.48                     | 0.44              |
| 1:A1:379:ILE:CD1  | 1:A1:390:ILE:HD12  | 2.41                     | 0.44              |
| 2:B1:154:ASN:O    | 2:B1:155:PRO:C     | 2.60                     | 0.44              |
| 2:B1:367:GLY:O    | 2:B1:368:TYR:C     | 2.59                     | 0.44              |
| 3:C1:147:THR:CG2  | 3:C1:165:TRP:NE1   | 2.78                     | 0.44              |
| 3:C1:338:ILE:HA   | 3:C1:341:GLN:HG3   | 1.99                     | 0.44              |
| 6:F1:37:ILE:CD1   | 6:F1:43:VAL:HG22   | 2.47                     | 0.44              |
| 1:M1:8:LEU:HD11   | 1:M1:396:GLU:HG3   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:49:SER:N      | 1:M1:52:ASN:OD1    | 2.41                     | 0.44              |
| 1:M1:349:ALA:O     | 1:M1:408:ARG:CZ    | 2.65                     | 0.44              |
| 2:N1:140:LEU:O     | 2:N1:142:PRO:N     | 2.51                     | 0.44              |
| 3:O1:136:GLY:O     | 3:O1:137:GLN:C     | 2.60                     | 0.44              |
| 3:O1:156:ILE:HG13  | 3:O1:157:GLY:N     | 2.29                     | 0.44              |
| 4:P1:139:THR:HB    | 8:T1:54:CYS:SG     | 2.58                     | 0.44              |
| 10:V1:4:THR:CG2    | 10:V1:6:THR:OG1    | 2.66                     | 0.44              |
| 10:V1:24:ILE:O     | 10:V1:25:VAL:C     | 2.61                     | 0.44              |
| 10:V1:57:HIS:O     | 10:V1:60:GLU:HG2   | 2.18                     | 0.44              |
| 12:22:48:HIS:HD2   | 16:72:171:ILE:HG23 | 1.83                     | 0.44              |
| 14:42:55:LEU:HD22  | 34:Q2:171:THR:HG22 | 1.99                     | 0.44              |
| 19:A2:111:LYS:HD2  | 33:P2:53:TYR:CZ    | 2.52                     | 0.44              |
| 22:D2:174:ASP:OD1  | 22:D2:182:TYR:OH   | 2.35                     | 0.44              |
| 50:i2:52:VAL:HA    | 50:i2:55:TRP:HB2   | 2.00                     | 0.44              |
| 52:12:254:LEU:HA   | 52:12:257:ILE:HD12 | 1.99                     | 0.44              |
| 53:62:448:PRO:HA   | 53:62:451:ILE:HB   | 2.00                     | 0.44              |
| 57:B3:59:GLN:CA    | 57:B3:62:GLU:HB2   | 2.46                     | 0.44              |
| 59:D3:40:LEU:HD22  | 59:D3:59:LEU:CD1   | 2.47                     | 0.44              |
| 1:A1:33:PRO:O      | 1:A1:103:SER:HB3   | 2.17                     | 0.44              |
| 1:A1:51:LYS:C      | 1:A1:53:ASN:H      | 2.25                     | 0.44              |
| 1:A1:358:LYS:HD2   | 1:A1:402:VAL:HB    | 1.98                     | 0.44              |
| 1:A1:426:GLY:HA2   | 1:A1:428:ILE:HG13  | 1.84                     | 0.44              |
| 2:B1:56:ARG:HH22   | 2:B1:318:ASP:CG    | 2.22                     | 0.44              |
| 2:B1:59:ASN:CG     | 2:B1:60:SER:N      | 2.74                     | 0.44              |
| 2:B1:264:ILE:HG22  | 2:B1:317:SER:HA    | 1.99                     | 0.44              |
| 3:C1:11:MET:HE3    | 3:C1:11:MET:HB3    | 1.67                     | 0.44              |
| 3:C1:156:ILE:HG12  | 3:C1:157:GLY:N     | 2.29                     | 0.44              |
| 4:D1:233:ARG:CG    | 7:G1:17:SER:HB3    | 2.48                     | 0.44              |
| 1:M1:324:PHE:CG    | 1:M1:334:MET:HG2   | 2.52                     | 0.44              |
| 2:N1:161:GLU:O     | 2:N1:162:ASN:C     | 2.60                     | 0.44              |
| 4:P1:28:ARG:HD2    | 4:P1:185:ASP:OD2   | 2.17                     | 0.44              |
| 4:P1:161:ALA:O     | 4:P1:163:PRO:HD3   | 2.18                     | 0.44              |
| 4:P1:237:TYR:HB2   | 6:R1:60:PHE:CE1    | 2.53                     | 0.44              |
| 5:Q1:186:GLU:O     | 5:Q1:186:GLU:CG    | 2.66                     | 0.44              |
| 9:U1:72:VAL:CB     | 9:U1:73:PRO:CD     | 2.76                     | 0.44              |
| 72:22:401:3PE:H281 | 51:j2:43:LEU:HD13  | 2.00                     | 0.44              |
| 19:A2:422:TRP:HA   | 19:A2:427:LEU:HB3  | 1.99                     | 0.44              |
| 20:B2:221:ARG:NH1  | 22:D2:95:GLU:OE2   | 2.51                     | 0.44              |
| 22:D2:175:ARG:HG2  | 35:R2:48:ARG:HH21  | 1.83                     | 0.44              |
| 25:G2:108:GLU:HG2  | 25:G2:113:GLY:HA2  | 1.99                     | 0.44              |
| 26:H2:9:ARG:NH2    | 51:j2:12:GLN:OE1   | 2.50                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:Q2:59:GLU:HA   | 34:Q2:62:LEU:HD13  | 2.00                     | 0.44              |
| 77:R2:601:NAP:O4D | 77:R2:601:NAP:C2N  | 2.65                     | 0.44              |
| 49:h2:81:ALA:HA   | 49:h2:84:ILE:HD12  | 1.99                     | 0.44              |
| 50:i2:51:SER:O    | 50:i2:55:TRP:N     | 2.46                     | 0.44              |
| 60:E3:70:VAL:HG12 | 60:E3:71:VAL:N     | 2.31                     | 0.44              |
| 1:A1:32:GLN:HE22  | 2:B1:373:GLU:HA    | 1.83                     | 0.44              |
| 1:A1:385:THR:HG22 | 1:A1:386:TYR:CD1   | 2.52                     | 0.44              |
| 2:B1:24:LEU:HG    | 2:B1:38:LEU:CD1    | 2.31                     | 0.44              |
| 2:B1:55:SER:HG    | 2:B1:102:ARG:HG2   | 1.83                     | 0.44              |
| 2:B1:211:VAL:HG12 | 2:B1:212:SER:N     | 2.32                     | 0.44              |
| 3:C1:103:TYR:CE1  | 3:C1:322:GLN:HG3   | 2.53                     | 0.44              |
| 3:C1:276:PHE:CE2  | 3:C1:297:SER:OG    | 2.68                     | 0.44              |
| 8:H1:69:VAL:O     | 8:H1:73:LEU:HB3    | 2.18                     | 0.44              |
| 1:M1:245:GLU:C    | 1:M1:247:GLY:N     | 2.76                     | 0.44              |
| 3:O1:30:TRP:HA    | 3:O1:33:PHE:CE2    | 2.52                     | 0.44              |
| 4:P1:27:ARG:NH1   | 10:V1:58:LYS:HE3   | 2.33                     | 0.44              |
| 4:P1:50:HIS:CE1   | 4:P1:91:PHE:HZ     | 2.33                     | 0.44              |
| 4:P1:131:LEU:CD2  | 4:P1:163:PRO:HB3   | 2.48                     | 0.44              |
| 5:Q1:99:ARG:NH1   | 5:Q1:148:ALA:HB1   | 2.32                     | 0.44              |
| 14:42:16:TRP:HA   | 14:42:93:LYS:HD3   | 1.99                     | 0.44              |
| 14:42:25:VAL:HG23 | 49:h2:89:VAL:HG11  | 1.99                     | 0.44              |
| 15:52:51:SER:HA   | 26:H2:32:ARG:HE    | 1.83                     | 0.44              |
| 17:82:219:LYS:NZ  | 25:G2:172:VAL:O    | 2.42                     | 0.44              |
| 17:82:383:THR:CG2 | 19:A2:75:CYS:CA    | 2.82                     | 0.44              |
| 52:12:39:VAL:HG13 | 52:12:40:VAL:HG13  | 1.99                     | 0.44              |
| 53:62:135:ASN:HA  | 53:62:198:LEU:HD12 | 1.99                     | 0.44              |
| 1:A1:277:ILE:HB   | 1:A1:309:THR:HG21  | 2.00                     | 0.44              |
| 2:B1:135:TRP:CE2  | 6:R1:49:ARG:HD3    | 2.53                     | 0.44              |
| 3:C1:233:LEU:HD12 | 3:C1:233:LEU:HA    | 1.80                     | 0.44              |
| 4:D1:7:PRO:HG3    | 4:D1:126:TYR:CA    | 2.43                     | 0.44              |
| 4:D1:10:TYR:HD1   | 8:H1:74:PHE:CD1    | 2.36                     | 0.44              |
| 4:D1:178:THR:HB   | 4:D1:181:GLN:CG    | 2.42                     | 0.44              |
| 5:E1:15:ARG:O     | 5:E1:16:PRO:C      | 2.61                     | 0.44              |
| 6:F1:106:GLU:OE1  | 6:F1:109:LYS:HE2   | 2.17                     | 0.44              |
| 1:M1:287:GLY:O    | 1:M1:290:LEU:HG    | 2.18                     | 0.44              |
| 2:N1:433:THR:HA   | 2:N1:434:PRO:HD2   | 1.58                     | 0.44              |
| 4:P1:26:ILE:CG2   | 4:P1:54:VAL:HG13   | 2.46                     | 0.44              |
| 4:P1:34:LYS:O     | 4:P1:34:LYS:HG2    | 2.18                     | 0.44              |
| 5:Q1:81:ILE:HD11  | 5:Q1:132:TRP:HH2   | 1.82                     | 0.44              |
| 5:Q1:136:ILE:O    | 5:Q1:138:VAL:N     | 2.49                     | 0.44              |
| 35:R2:143:ASP:O   | 35:R2:147:LYS:N    | 2.43                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:62:73:THR:O     | 54:g2:104:ASN:ND2  | 2.49                     | 0.44              |
| 57:B3:162:SER:HB2  | 57:B3:198:GLU:HB2  | 1.99                     | 0.44              |
| 1:A1:198:ALA:O     | 1:A1:199:ALA:CB    | 2.63                     | 0.44              |
| 1:A1:293:PRO:HA    | 1:A1:296:SER:OG    | 2.17                     | 0.44              |
| 2:B1:181:TYR:CD1   | 2:B1:181:TYR:C     | 2.96                     | 0.44              |
| 2:B1:258:VAL:HG11  | 2:B1:321:LEU:HD22  | 2.00                     | 0.44              |
| 2:B1:275:LEU:HD11  | 2:B1:279:LEU:HD12  | 1.99                     | 0.44              |
| 2:B1:334:GLY:O     | 2:B1:335:ASP:C     | 2.59                     | 0.44              |
| 3:C1:357:LEU:HD12  | 3:C1:361:LEU:HG    | 2.00                     | 0.44              |
| 4:D1:120:ARG:HH11  | 4:D1:120:ARG:HG2   | 1.82                     | 0.44              |
| 7:G1:26:PHE:N      | 7:G1:27:PRO:HD3    | 2.33                     | 0.44              |
| 1:M1:385:THR:HB    | 1:M1:386:TYR:CD1   | 2.53                     | 0.44              |
| 2:N1:160:ILE:HD11  | 2:N1:325:TYR:CE2   | 2.53                     | 0.44              |
| 3:O1:88:SER:O      | 3:O1:89:MET:C      | 2.61                     | 0.44              |
| 3:O1:160:LEU:O     | 3:O1:160:LEU:HD12  | 2.18                     | 0.44              |
| 3:O1:197:LEU:HD12  | 3:O1:197:LEU:HA    | 1.77                     | 0.44              |
| 4:P1:35:GLN:OE1    | 4:P1:35:GLN:HA     | 2.18                     | 0.44              |
| 4:P1:68:VAL:CG1    | 4:P1:92:PRO:HG2    | 2.47                     | 0.44              |
| 5:Q1:171:ILE:HB    | 5:Q1:178:LEU:O     | 2.17                     | 0.44              |
| 7:S1:26:PHE:N      | 7:S1:27:PRO:HD3    | 2.32                     | 0.44              |
| 10:V1:51:LEU:O     | 10:V1:52:TRP:C     | 2.61                     | 0.44              |
| 17:82:124:THR:HG22 | 17:82:126:LYS:H    | 1.83                     | 0.44              |
| 17:82:445:GLU:O    | 17:82:449:ARG:NH1  | 2.51                     | 0.44              |
| 19:A2:634:LEU:HA   | 19:A2:635:PRO:HD3  | 1.81                     | 0.44              |
| 35:R2:235:THR:HA   | 35:R2:236:VAL:HA   | 1.57                     | 0.44              |
| 35:R2:269:SER:HA   | 35:R2:270:ARG:HA   | 1.64                     | 0.44              |
| 44:a2:113:GLU:O    | 44:a2:117:GLN:N    | 2.46                     | 0.44              |
| 53:62:319:ILE:HG22 | 53:62:321:GLN:HG2  | 1.99                     | 0.44              |
| 2:B1:262:ALA:CB    | 2:B1:268:GLU:HB3   | 2.48                     | 0.43              |
| 2:B1:285:VAL:HG12  | 2:B1:288:GLY:HA3   | 1.98                     | 0.43              |
| 3:C1:242:LEU:HD21  | 3:C1:250:LEU:HD22  | 1.99                     | 0.43              |
| 3:C1:254:ASP:HB3   | 4:D1:119:ALA:O     | 2.18                     | 0.43              |
| 3:C1:294:LEU:O     | 3:C1:297:SER:HB3   | 2.17                     | 0.43              |
| 69:C1:401:HEM:CMB  | 69:C1:401:HEM:HBB2 | 2.48                     | 0.43              |
| 4:D1:72:ASP:OD2    | 4:D1:92:PRO:HB2    | 2.18                     | 0.43              |
| 4:D1:131:LEU:HD13  | 4:D1:164:ILE:CD1   | 2.48                     | 0.43              |
| 4:D1:161:ALA:O     | 4:D1:163:PRO:CD    | 2.66                     | 0.43              |
| 1:M1:85:HIS:HA     | 2:N1:284:HIS:O     | 2.18                     | 0.43              |
| 1:M1:152:TYR:OH    | 1:M1:243:HIS:CD2   | 2.71                     | 0.43              |
| 2:N1:62:ASN:ND2    | 2:N1:65:THR:CB     | 2.81                     | 0.43              |
| 3:O1:101:GLY:O     | 3:O1:107:TYR:HD2   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O1:327:ALA:HA    | 7:S1:51:PRO:HB3    | 1.99                     | 0.43              |
| 4:P1:102:ARG:HE    | 4:P1:109:LEU:HB2   | 1.83                     | 0.43              |
| 4:P1:210:LEU:O     | 4:P1:211:MET:C     | 2.60                     | 0.43              |
| 8:T1:58:LEU:CD1    | 8:T1:62:LEU:HG     | 2.48                     | 0.43              |
| 14:42:76:MET:HG2   | 14:42:231:LEU:HD12 | 1.99                     | 0.43              |
| 17:82:284:ASN:HD22 | 18:92:228:ALA:HB3  | 1.83                     | 0.43              |
| 19:A2:250:SER:OG   | 19:A2:251:ILE:N    | 2.51                     | 0.43              |
| 27:I2:89:GLY:H     | 27:I2:96:HIS:CE1   | 2.35                     | 0.43              |
| 42:Y2:47:TYR:HD2   | 43:Z2:16:LEU:HD12  | 1.82                     | 0.43              |
| 58:C3:19:THR:CG2   | 58:C3:53:THR:OG1   | 2.66                     | 0.43              |
| 1:A1:16:VAL:HG11   | 1:A1:388:ARG:HB2   | 1.99                     | 0.43              |
| 2:B1:257:LEU:HD22  | 2:B1:424:MET:HE2   | 2.00                     | 0.43              |
| 3:C1:8:HIS:HB2     | 3:C1:9:PRO:HD2     | 2.00                     | 0.43              |
| 3:C1:245:PHE:CE1   | 4:D1:17:LEU:HB3    | 2.53                     | 0.43              |
| 5:E1:33:LYS:HA     | 7:G1:21:PHE:HE2    | 1.82                     | 0.43              |
| 7:G1:27:PRO:O      | 7:G1:28:HIS:C      | 2.62                     | 0.43              |
| 9:I1:64:LEU:HG     | 9:I1:65:VAL:HG23   | 1.99                     | 0.43              |
| 1:M1:64:PHE:HE1    | 1:M1:86:LEU:CD1    | 2.31                     | 0.43              |
| 1:M1:252:HIS:CD2   | 1:M1:325:VAL:HG22  | 2.53                     | 0.43              |
| 2:N1:53:ALA:O      | 2:N1:105:MET:HB2   | 2.17                     | 0.43              |
| 2:N1:83:PHE:CZ     | 2:N1:87:ARG:HG3    | 2.53                     | 0.43              |
| 2:N1:99:THR:O      | 2:N1:106:ALA:N     | 2.51                     | 0.43              |
| 2:N1:109:VAL:O     | 2:N1:109:VAL:CG1   | 2.66                     | 0.43              |
| 2:N1:129:ALA:O     | 2:N1:130:PRO:C     | 2.58                     | 0.43              |
| 2:N1:206:LEU:C     | 2:N1:207:ILE:HG12  | 2.43                     | 0.43              |
| 3:O1:31:TRP:CD2    | 3:O1:100:ARG:HD2   | 2.53                     | 0.43              |
| 3:O1:282:ARG:O     | 3:O1:283:SER:C     | 2.59                     | 0.43              |
| 3:O1:316:MET:HE2   | 3:O1:317:PHE:HE1   | 1.77                     | 0.43              |
| 4:P1:12:TRP:O      | 4:P1:13:SER:C      | 2.61                     | 0.43              |
| 5:Q1:150:ALA:CB    | 5:Q1:157:TYR:HB2   | 2.48                     | 0.43              |
| 5:Q1:153:PHE:HE1   | 5:Q1:173:LYS:CG    | 2.25                     | 0.43              |
| 5:Q1:185:TYR:HB3   | 5:Q1:195:VAL:HA    | 2.00                     | 0.43              |
| 19:A2:35:PHE:HB3   | 19:A2:38:GLY:HA2   | 2.00                     | 0.43              |
| 19:A2:380:ASP:OD2  | 29:K2:45:LYS:HE3   | 2.18                     | 0.43              |
| 52:12:75:PRO:CB    | 52:12:223:PHE:CE1  | 3.02                     | 0.43              |
| 58:C3:63:ARG:HA    | 58:C3:67:PHE:CD2   | 2.53                     | 0.43              |
| 65:J3:3:ASN:ND2    | 65:J3:5:VAL:HG13   | 2.33                     | 0.43              |
| 67:L3:22:LEU:HD23  | 67:L3:22:LEU:HA    | 1.83                     | 0.43              |
| 1:A1:347:THR:HA    | 11:K1:16:ASN:HD22  | 1.84                     | 0.43              |
| 3:C1:7:SER:O       | 3:C1:8:HIS:O       | 2.36                     | 0.43              |
| 3:C1:107:TYR:CE2   | 3:C1:305:PRO:HA    | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C1:170:VAL:CG1  | 3:C1:174:THR:CG2   | 2.89                     | 0.43              |
| 4:D1:138:PRO:CG   | 8:H1:55:THR:HA     | 2.48                     | 0.43              |
| 1:M1:64:PHE:CD1   | 1:M1:86:LEU:HG     | 2.51                     | 0.43              |
| 1:M1:211:LEU:HD12 | 1:M1:211:LEU:O     | 2.18                     | 0.43              |
| 2:N1:222:GLN:HB3  | 2:N1:223:PHE:CD2   | 2.53                     | 0.43              |
| 3:O1:56:THR:HG22  | 3:O1:57:SER:N      | 2.34                     | 0.43              |
| 5:Q1:29:SER:OG    | 5:Q1:32:ARG:HD3    | 2.17                     | 0.43              |
| 14:42:368:ALA:HB1 | 14:42:374:ASN:HB2  | 1.99                     | 0.43              |
| 45:b2:68:LEU:H    | 45:b2:71:LEU:HD13  | 1.82                     | 0.43              |
| 52:12:20:LEU:O    | 52:12:24:GLU:N     | 2.49                     | 0.43              |
| 58:C3:60:ASP:O    | 58:C3:64:GLU:HG3   | 2.19                     | 0.43              |
| 1:A1:7:ALA:O      | 1:A1:8:LEU:C       | 2.60                     | 0.43              |
| 1:A1:21:ASN:CB    | 1:A1:217:SER:CB    | 2.89                     | 0.43              |
| 2:B1:346:THR:O    | 2:B1:347:ILE:C     | 2.60                     | 0.43              |
| 3:C1:32:ASN:O     | 3:C1:36:LEU:HG     | 2.18                     | 0.43              |
| 3:C1:192:ILE:HD13 | 3:C1:192:ILE:H     | 1.82                     | 0.43              |
| 3:C1:206:ASN:ND2  | 3:C1:207:ASN:N     | 2.60                     | 0.43              |
| 3:C1:269:LYS:HA   | 3:C1:270:PRO:HD3   | 1.81                     | 0.43              |
| 1:M1:19:LEU:HB2   | 1:M1:23:LEU:HB3    | 2.00                     | 0.43              |
| 1:M1:75:LEU:HD21  | 1:M1:116:ILE:HG12  | 2.00                     | 0.43              |
| 1:M1:292:SER:O    | 1:M1:295:ALA:N     | 2.52                     | 0.43              |
| 1:M1:381:ARG:HA   | 1:M1:384:LEU:HD12  | 1.99                     | 0.43              |
| 2:N1:182:ARG:NH1  | 2:N1:185:LYS:CG    | 2.79                     | 0.43              |
| 3:O1:25:SER:HB2   | 3:O1:26:ASN:H      | 1.30                     | 0.43              |
| 3:O1:183:PHE:CD1  | 3:O1:183:PHE:O     | 2.72                     | 0.43              |
| 3:O1:227:LYS:CG   | 4:P1:223:LYS:NZ    | 2.82                     | 0.43              |
| 3:O1:280:ILE:HD13 | 3:O1:335:LEU:CD2   | 2.44                     | 0.43              |
| 4:P1:82:MET:HE2   | 4:P1:86:LYS:HZ3    | 1.82                     | 0.43              |
| 4:P1:204:MET:O    | 4:P1:205:GLY:C     | 2.60                     | 0.43              |
| 5:Q1:121:GLN:O    | 5:Q1:170:ARG:HD3   | 2.18                     | 0.43              |
| 5:Q1:122:HIS:O    | 5:Q1:123:ASP:C     | 2.62                     | 0.43              |
| 7:S1:68:LYS:HD3   | 7:S1:72:LYS:HE3    | 2.01                     | 0.43              |
| 12:22:146:PHE:HE1 | 12:22:195:PRO:HA   | 1.82                     | 0.43              |
| 14:42:198:ALA:HB2 | 72:42:502:3PE:H271 | 2.00                     | 0.43              |
| 17:82:378:SER:OG  | 19:A2:201:GLY:HA2  | 2.18                     | 0.43              |
| 74:82:501:FMN:H9  | 74:82:501:FMN:H1'1 | 1.68                     | 0.43              |
| 20:B2:85:GLY:C    | 20:B2:87:GLN:H     | 2.26                     | 0.43              |
| 20:B2:97:LEU:C    | 20:B2:97:LEU:HD13  | 2.43                     | 0.43              |
| 20:B2:118:ARG:HD3 | 22:D2:163:TYR:CZ   | 2.54                     | 0.43              |
| 21:C2:157:SER:HB3 | 21:C2:180:PHE:HB3  | 2.01                     | 0.43              |
| 23:E2:197:TRP:HB3 | 38:U2:84:PRO:HB2   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:R2:177:SER:HA   | 35:R2:178:SER:HA  | 1.68                     | 0.43              |
| 50:i2:43:LYS:HA    | 50:i2:46:LEU:HD12 | 1.99                     | 0.43              |
| 52:12:178:ALA:HB1  | 52:12:181:LEU:HB2 | 2.00                     | 0.43              |
| 58:C3:19:THR:HG22  | 58:C3:53:THR:OG1  | 2.18                     | 0.43              |
| 1:A1:154:HIS:HE1   | 1:A1:314:TYR:OH   | 2.02                     | 0.43              |
| 2:B1:262:ALA:HB2   | 2:B1:272:PHE:CE2  | 2.53                     | 0.43              |
| 3:C1:226:ILE:O     | 3:C1:227:LYS:C    | 2.61                     | 0.43              |
| 6:F1:70:MET:HE2    | 6:F1:70:MET:HB3   | 1.60                     | 0.43              |
| 1:M1:106:LEU:HA    | 1:M1:109:ALA:HB3  | 2.01                     | 0.43              |
| 1:M1:158:PHE:O     | 1:M1:164:ALA:HB2  | 2.18                     | 0.43              |
| 2:N1:47:ILE:CG2    | 2:N1:48:GLY:H     | 2.31                     | 0.43              |
| 2:N1:162:ASN:ND2   | 2:N1:244:ILE:HG21 | 2.33                     | 0.43              |
| 2:N1:204:MET:HE1   | 2:N1:224:LEU:HB3  | 2.00                     | 0.43              |
| 3:O1:276:PHE:HE2   | 3:O1:297:SER:OG   | 2.00                     | 0.43              |
| 3:O1:373:GLU:HB3   | 6:R1:20:TYR:OH    | 2.18                     | 0.43              |
| 4:P1:28:ARG:O      | 4:P1:29:GLY:C     | 2.61                     | 0.43              |
| 4:P1:131:LEU:HD22  | 4:P1:163:PRO:CB   | 2.48                     | 0.43              |
| 5:Q1:122:HIS:HB3   | 5:Q1:125:GLU:CG   | 2.48                     | 0.43              |
| 17:82:177:TYR:O    | 24:F2:96:ARG:NH1  | 2.52                     | 0.43              |
| 28:J2:68:ASN:ND2   | 34:Q2:19:LYS:O    | 2.51                     | 0.43              |
| 36:S2:73:HIS:NE2   | 36:S2:148:GLU:OE2 | 2.41                     | 0.43              |
| 41:X2:21:VAL:HA    | 41:X2:24:TYR:HB3  | 1.99                     | 0.43              |
| 43:Z2:65:GLY:O     | 43:Z2:70:GLY:N    | 2.48                     | 0.43              |
| 44:a2:87:SER:O     | 53:62:557:TRP:NE1 | 2.52                     | 0.43              |
| 56:A3:353:LEU:HD12 | 56:A3:353:LEU:HA  | 1.91                     | 0.43              |
| 1:A1:428:ILE:CG2   | 1:A1:431:LEU:HD22 | 2.47                     | 0.43              |
| 2:B1:245:ARG:HH11  | 2:B1:245:ARG:HD3  | 1.53                     | 0.43              |
| 2:B1:259:ALA:O     | 2:B1:260:GLU:C    | 2.61                     | 0.43              |
| 3:C1:34:GLY:O      | 3:C1:37:LEU:CB    | 2.57                     | 0.43              |
| 3:C1:89:MET:O      | 3:C1:90:PHE:C     | 2.62                     | 0.43              |
| 3:C1:122:THR:CG2   | 3:C1:189:ILE:CG1  | 2.96                     | 0.43              |
| 4:D1:220:TYR:CD2   | 7:G1:26:PHE:CZ    | 3.06                     | 0.43              |
| 10:J1:31:PHE:CD1   | 10:J1:31:PHE:C    | 2.96                     | 0.43              |
| 1:M1:4:TYR:CD1     | 2:N1:43:PRO:HB3   | 2.53                     | 0.43              |
| 1:M1:134:ILE:HA    | 1:M1:134:ILE:HD13 | 1.53                     | 0.43              |
| 1:M1:145:MET:CE    | 1:M1:248:LEU:HD12 | 2.48                     | 0.43              |
| 1:M1:153:LEU:CD2   | 1:M1:319:LEU:HD13 | 2.48                     | 0.43              |
| 1:M1:271:GLN:O     | 1:M1:272:VAL:C    | 2.59                     | 0.43              |
| 1:M1:366:VAL:HG11  | 2:N1:44:ALA:HB2   | 1.99                     | 0.43              |
| 2:N1:207:ILE:CD1   | 2:N1:383:GLY:CA   | 2.93                     | 0.43              |
| 3:O1:207:ASN:OD1   | 3:O1:207:ASN:O    | 2.37                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:O1:319:PRO:O     | 3:O1:320:LEU:C    | 2.61                     | 0.43              |
| 4:P1:7:PRO:HB3     | 4:P1:125:ASP:HB3  | 2.01                     | 0.43              |
| 4:P1:165:TYR:CE1   | 4:P1:168:VAL:HA   | 2.54                     | 0.43              |
| 4:P1:229:VAL:HG12  | 4:P1:233:ARG:NE   | 2.32                     | 0.43              |
| 5:Q1:122:HIS:ND1   | 5:Q1:124:LEU:N    | 2.57                     | 0.43              |
| 10:V1:44:GLU:O     | 10:V1:45:HIS:C    | 2.62                     | 0.43              |
| 14:42:34:ILE:O     | 14:42:37:THR:OG1  | 2.33                     | 0.43              |
| 17:82:418:GLN:HE21 | 19:A2:115:GLY:C   | 2.21                     | 0.43              |
| 19:A2:560:LEU:HD12 | 19:A2:561:PRO:HD2 | 1.99                     | 0.43              |
| 20:B2:267:ILE:O    | 20:B2:271:ARG:N   | 2.49                     | 0.43              |
| 36:S2:280:HIS:O    | 36:S2:283:ARG:N   | 2.51                     | 0.43              |
| 54:g2:162:ARG:HA   | 54:g2:165:ALA:HB3 | 2.00                     | 0.43              |
| 57:B3:63:THR:HA    | 57:B3:66:THR:HG22 | 2.00                     | 0.43              |
| 58:C3:40:MET:O     | 58:C3:41:THR:C    | 2.62                     | 0.43              |
| 60:E3:27:TRP:CH2   | 61:F3:86:GLY:HA2  | 2.54                     | 0.43              |
| 62:G3:42:ARG:HG3   | 62:G3:42:ARG:NH1  | 2.32                     | 0.43              |
| 64:I3:21:ILE:O     | 64:I3:25:PHE:HD2  | 2.02                     | 0.43              |
| 64:I3:68:ILE:HG13  | 64:I3:69:PHE:N    | 2.33                     | 0.43              |
| 65:J3:30:ILE:HG13  | 65:J3:31:LEU:N    | 2.33                     | 0.43              |
| 66:K3:44:PRO:HA    | 66:K3:47:ARG:NH1  | 2.34                     | 0.43              |
| 2:B1:348:ALA:CB    | 2:B1:418:VAL:HG21 | 2.49                     | 0.43              |
| 3:C1:92:ILE:HG12   | 3:C1:272:TRP:CH2  | 2.54                     | 0.43              |
| 3:C1:109:PHE:HE2   | 3:C1:203:THR:HG1  | 1.58                     | 0.43              |
| 3:C1:200:LEU:HD13  | 69:C1:402:HEM:CAD | 2.49                     | 0.43              |
| 3:C1:342:PRO:HG2   | 7:G1:66:PHE:CZ    | 2.53                     | 0.43              |
| 10:J1:52:TRP:CG    | 10:J1:53:LYS:N    | 2.86                     | 0.43              |
| 1:M1:64:PHE:HE2    | 1:M1:88:ALA:HB2   | 1.81                     | 0.43              |
| 2:N1:283:PRO:HG3   | 9:U1:55:LEU:CG    | 2.49                     | 0.43              |
| 2:N1:332:SER:O     | 2:N1:333:ALA:C    | 2.60                     | 0.43              |
| 2:N1:334:GLY:O     | 2:N1:335:ASP:C    | 2.60                     | 0.43              |
| 2:N1:357:VAL:O     | 2:N1:360:ALA:HB3  | 2.18                     | 0.43              |
| 3:O1:257:THR:O     | 3:O1:258:PRO:C    | 2.62                     | 0.43              |
| 4:P1:91:PHE:HA     | 4:P1:92:PRO:HD3   | 1.60                     | 0.43              |
| 4:P1:195:GLU:HA    | 4:P1:196:PRO:HD2  | 1.73                     | 0.43              |
| 5:Q1:14:ARG:HA     | 7:S1:23:GLN:HA    | 2.01                     | 0.43              |
| 5:Q1:141:HIS:CE1   | 5:Q1:175:PRO:HG2  | 2.54                     | 0.43              |
| 9:U1:70:LEU:CD2    | 9:U1:73:PRO:CD    | 2.92                     | 0.43              |
| 19:A2:650:SER:OG   | 19:A2:652:ASN:OD1 | 2.30                     | 0.43              |
| 20:B2:238:LEU:HD23 | 39:V2:10:MET:HE1  | 1.99                     | 0.43              |
| 20:B2:278:VAL:HG12 | 20:B2:283:ALA:HB2 | 2.00                     | 0.43              |
| 27:I2:105:LYS:HB3  | 27:I2:105:LYS:HE2 | 1.82                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:12:65:THR:OG1   | 52:12:124:ASN:ND2  | 2.49                     | 0.43              |
| 53:62:15:LEU:HD21  | 53:62:125:LEU:HD22 | 1.99                     | 0.43              |
| 56:A3:513:LEU:HD12 | 56:A3:513:LEU:HA   | 1.65                     | 0.43              |
| 57:B3:52:HIS:CD2   | 60:E3:40:ASP:HB2   | 2.54                     | 0.43              |
| 58:C3:148:HIS:CE1  | 58:C3:152:MET:HE3  | 2.54                     | 0.43              |
| 63:H3:57:ARG:HB3   | 63:H3:57:ARG:NH1   | 2.31                     | 0.43              |
| 1:A1:19:LEU:HD22   | 1:A1:214:LYS:NZ    | 2.34                     | 0.43              |
| 2:B1:110:GLU:O     | 2:B1:111:CYS:HB3   | 2.18                     | 0.43              |
| 2:B1:122:PHE:O     | 2:B1:126:VAL:HG23  | 2.18                     | 0.43              |
| 2:B1:369:LEU:O     | 2:B1:370:MET:C     | 2.61                     | 0.43              |
| 3:C1:9:PRO:CG      | 3:C1:12:LYS:HB2    | 2.45                     | 0.43              |
| 3:C1:37:LEU:CD1    | 3:C1:97:HIS:CD2    | 3.02                     | 0.43              |
| 3:C1:71:ARG:HB3    | 4:D1:49:ARG:HH22   | 1.84                     | 0.43              |
| 3:C1:107:TYR:HE2   | 3:C1:305:PRO:HA    | 1.83                     | 0.43              |
| 3:C1:196:HIS:HE1   | 69:C1:402:HEM:C1D  | 2.37                     | 0.43              |
| 3:C1:218:ILE:CG2   | 3:C1:219:PRO:N     | 2.82                     | 0.43              |
| 4:D1:41:HIS:CD2    | 70:D1:301:HEC:NB   | 2.84                     | 0.43              |
| 6:F1:49:ARG:NH2    | 6:F1:100:GLU:OE2   | 2.47                     | 0.43              |
| 2:N1:47:ILE:HB     | 2:N1:109:VAL:CG1   | 2.49                     | 0.43              |
| 2:N1:363:LYS:O     | 2:N1:364:LEU:C     | 2.61                     | 0.43              |
| 2:N1:372:VAL:O     | 2:N1:372:VAL:CG1   | 2.67                     | 0.43              |
| 3:O1:119:LEU:CD1   | 3:O1:192:ILE:CG2   | 2.97                     | 0.43              |
| 3:O1:338:ILE:HA    | 3:O1:341:GLN:CG    | 2.49                     | 0.43              |
| 4:P1:150:ASN:OD1   | 4:P1:151:PRO:HD2   | 2.19                     | 0.43              |
| 4:P1:220:TYR:O     | 4:P1:223:LYS:N     | 2.52                     | 0.43              |
| 6:R1:94:LEU:O      | 6:R1:98:ILE:HG13   | 2.19                     | 0.43              |
| 16:72:25:SER:O     | 16:72:27:ILE:N     | 2.47                     | 0.43              |
| 19:A2:162:ASP:O    | 27:I2:105:LYS:CE   | 2.66                     | 0.43              |
| 19:A2:251:ILE:HB   | 19:A2:606:THR:HG22 | 2.01                     | 0.43              |
| 19:A2:313:LEU:N    | 38:U2:142:THR:CA   | 2.78                     | 0.43              |
| 20:B2:398:THR:OG1  | 20:B2:399:ALA:N    | 2.52                     | 0.43              |
| 42:Y2:57:GLN:HE22  | 53:62:445:GLU:HB3  | 1.83                     | 0.43              |
| 58:C3:41:THR:O     | 58:C3:45:ILE:HG13  | 2.18                     | 0.43              |
| 1:A1:86:LEU:HD12   | 1:A1:98:TYR:O      | 2.19                     | 0.43              |
| 1:A1:86:LEU:CD1    | 1:A1:99:ILE:HG12   | 2.44                     | 0.43              |
| 1:A1:152:TYR:O     | 1:A1:153:LEU:C     | 2.57                     | 0.43              |
| 3:C1:336:THR:O     | 3:C1:336:THR:HG22  | 2.18                     | 0.43              |
| 7:G1:36:ASN:OD1    | 7:G1:39:ARG:NE     | 2.52                     | 0.43              |
| 8:H1:15:ASP:HB2    | 8:H1:16:PRO:HD3    | 2.01                     | 0.43              |
| 1:M1:73:ASN:O      | 1:M1:77:LYS:CD     | 2.66                     | 0.43              |
| 1:M1:281:ASP:HB3   | 1:M1:284:TYR:CD1   | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:349:ALA:HB3   | 1:M1:408:ARG:NE    | 2.34                     | 0.43              |
| 2:N1:67:HIS:HD2    | 2:N1:144:LEU:CD2   | 2.16                     | 0.43              |
| 3:O1:7:SER:O       | 3:O1:8:HIS:C       | 2.61                     | 0.43              |
| 3:O1:103:TYR:CE1   | 3:O1:322:GLN:HG3   | 2.53                     | 0.43              |
| 3:O1:230:LEU:O     | 3:O1:230:LEU:HG    | 2.17                     | 0.43              |
| 4:P1:5:LEU:HG      | 4:P1:152:TYR:CE1   | 2.54                     | 0.43              |
| 5:Q1:20:ASP:O      | 5:Q1:22:THR:N      | 2.52                     | 0.43              |
| 5:Q1:182:VAL:C     | 5:Q1:183:PRO:O     | 2.57                     | 0.43              |
| 6:R1:101:ARG:HG2   | 6:R1:105:GLU:OE2   | 2.19                     | 0.43              |
| 12:22:200:MET:HG2  | 12:22:341:PRO:HB3  | 2.01                     | 0.43              |
| 18:92:153:GLN:HG3  | 18:92:158:ILE:HG13 | 2.00                     | 0.43              |
| 19:A2:144:MET:HG2  | 20:B2:380:HIS:HD2  | 1.80                     | 0.43              |
| 23:E2:170:GLY:HA2  | 23:E2:171:PRO:HD3  | 1.78                     | 0.43              |
| 48:f2:35:ASP:HA    | 48:f2:38:ARG:HB3   | 2.01                     | 0.43              |
| 56:A3:70:VAL:HG11  | 56:A3:246:LEU:HD22 | 2.00                     | 0.43              |
| 58:C3:110:PRO:HB3  | 63:H3:30:TRP:CD2   | 2.54                     | 0.43              |
| 62:G3:5:LYS:CD     | 62:G3:6:GLY:N      | 2.81                     | 0.43              |
| 67:L3:41:ARG:HD2   | 68:M3:40:TYR:CZ    | 2.54                     | 0.43              |
| 1:A1:3:THR:O       | 1:A1:4:TYR:C       | 2.62                     | 0.43              |
| 1:A1:136:GLN:HE21  | 9:I1:50:LEU:HG     | 1.84                     | 0.43              |
| 1:A1:255:ILE:HD12  | 1:A1:335:MET:HE1   | 2.01                     | 0.43              |
| 1:A1:343:MET:H     | 1:A1:343:MET:HG2   | 1.34                     | 0.43              |
| 2:B1:295:LEU:O     | 2:B1:299:VAL:HG23  | 2.19                     | 0.43              |
| 3:C1:307:LEU:O     | 3:C1:308:HIS:C     | 2.62                     | 0.43              |
| 3:C1:368:THR:O     | 3:C1:369:ALA:C     | 2.62                     | 0.43              |
| 4:D1:21:LEU:CD1    | 4:D1:26:ILE:HD11   | 2.49                     | 0.43              |
| 1:M1:19:LEU:CD1    | 1:M1:214:LYS:HG2   | 2.48                     | 0.43              |
| 1:M1:213:GLN:CB    | 1:M1:215:HIS:CD2   | 3.02                     | 0.43              |
| 2:N1:70:ARG:HD2    | 9:U1:69:SER:HB3    | 2.01                     | 0.43              |
| 6:R1:87:LYS:HE2    | 6:R1:89:TYR:HB3    | 2.01                     | 0.43              |
| 8:T1:22:GLU:O      | 8:T1:23:GLN:C      | 2.60                     | 0.43              |
| 19:A2:140:GLN:HE22 | 20:B2:382:PHE:HE2  | 1.66                     | 0.43              |
| 21:C2:165:ALA:HB1  | 21:C2:169:GLU:HG3  | 2.00                     | 0.43              |
| 54:g2:76:GLU:HA    | 54:g2:77:CYS:HA    | 1.74                     | 0.43              |
| 57:B3:3:TYR:CD1    | 57:B3:3:TYR:N      | 2.87                     | 0.43              |
| 61:F3:53:THR:HG22  | 61:F3:54:ASN:OD1   | 2.19                     | 0.43              |
| 65:J3:36:MET:O     | 65:J3:40:LEU:HG    | 2.18                     | 0.43              |
| 1:A1:80:GLU:C      | 1:A1:82:MET:N      | 2.77                     | 0.42              |
| 1:A1:260:PRO:HG3   | 1:A1:414:TYR:OH    | 2.19                     | 0.42              |
| 1:A1:343:MET:CE    | 1:A1:416:TYR:HD2   | 2.17                     | 0.42              |
| 3:C1:157:GLY:O     | 3:C1:160:LEU:N     | 2.51                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:316:MET:HG2   | 3:C1:317:PHE:CD1   | 2.54                     | 0.42              |
| 4:D1:3:LEU:HD22    | 7:G1:70:LYS:HZ3    | 1.81                     | 0.42              |
| 4:D1:10:TYR:CE1    | 4:D1:128:PHE:CE2   | 3.07                     | 0.42              |
| 4:D1:116:ILE:CD1   | 4:D1:120:ARG:HG3   | 2.49                     | 0.42              |
| 4:D1:209:LEU:O     | 4:D1:210:LEU:C     | 2.62                     | 0.42              |
| 7:G1:44:CYS:O      | 7:G1:47:ARG:N      | 2.47                     | 0.42              |
| 11:K1:20:THR:HG23  | 11:K1:24:TRP:CD1   | 2.54                     | 0.42              |
| 1:M1:56:GLY:O      | 1:M1:57:TYR:C      | 2.59                     | 0.42              |
| 1:M1:283:THR:OG1   | 9:U1:74:ALA:HB3    | 2.19                     | 0.42              |
| 2:N1:24:LEU:H      | 2:N1:24:LEU:CD1    | 2.18                     | 0.42              |
| 2:N1:211:VAL:HG12  | 2:N1:212:SER:N     | 2.34                     | 0.42              |
| 2:N1:367:GLY:O     | 2:N1:368:TYR:C     | 2.61                     | 0.42              |
| 3:O1:211:ILE:HG22  | 3:O1:212:SER:N     | 2.34                     | 0.42              |
| 4:P1:94:PRO:HB2    | 4:P1:95:TYR:CD1    | 2.54                     | 0.42              |
| 12:22:63:GLN:HA    | 12:22:66:ALA:HB3   | 2.01                     | 0.42              |
| 12:22:257:LEU:HD23 | 12:22:257:LEU:HA   | 1.89                     | 0.42              |
| 17:82:160:GLY:HA2  | 17:82:199:ARG:HD2  | 2.00                     | 0.42              |
| 19:A2:605:GLN:HG3  | 19:A2:607:LYS:HZ2  | 1.84                     | 0.42              |
| 21:C2:86:LEU:HB2   | 21:C2:143:ILE:HG13 | 2.01                     | 0.42              |
| 21:C2:99:LEU:O     | 21:C2:103:ARG:N    | 2.52                     | 0.42              |
| 26:H2:96:PRO:HA    | 26:H2:97:HIS:HA    | 1.65                     | 0.42              |
| 36:S2:150:SER:OG   | 36:S2:151:ILE:N    | 2.51                     | 0.42              |
| 41:X2:14:VAL:HA    | 41:X2:17:PRO:HD2   | 2.01                     | 0.42              |
| 53:62:68:TRP:H     | 53:62:77:SER:HA    | 1.84                     | 0.42              |
| 64:I3:61:GLU:OE1   | 64:I3:64:ARG:NH1   | 2.51                     | 0.42              |
| 65:J3:11:LEU:HD23  | 65:J3:11:LEU:C     | 2.44                     | 0.42              |
| 1:A1:29:GLN:HA     | 1:A1:201:GLY:O     | 2.18                     | 0.42              |
| 1:A1:248:LEU:HA    | 1:A1:249:PRO:HD3   | 1.59                     | 0.42              |
| 1:A1:311:ASN:CG    | 1:A1:320:LEU:CD2   | 2.91                     | 0.42              |
| 2:B1:79:GLY:H      | 2:B1:125:ASN:HD22  | 1.67                     | 0.42              |
| 2:B1:286:LYS:HD3   | 2:B1:287:ARG:HH12  | 1.81                     | 0.42              |
| 3:C1:90:PHE:CZ     | 3:C1:123:VAL:HG21  | 2.54                     | 0.42              |
| 4:D1:214:LEU:O     | 4:D1:218:LEU:HG    | 2.19                     | 0.42              |
| 6:F1:87:LYS:HG3    | 6:F1:89:TYR:HB3    | 2.01                     | 0.42              |
| 6:F1:103:GLU:O     | 6:F1:104:ARG:C     | 2.62                     | 0.42              |
| 7:G1:39:ARG:HA     | 7:G1:42:ARG:HD2    | 2.00                     | 0.42              |
| 1:M1:38:GLY:HA3    | 1:M1:40:TRP:CZ3    | 2.49                     | 0.42              |
| 1:M1:277:ILE:HG22  | 1:M1:294:LEU:HD12  | 1.99                     | 0.42              |
| 2:N1:163:LEU:HD22  | 2:N1:256:ALA:HB1   | 2.01                     | 0.42              |
| 2:N1:264:ILE:HB    | 2:N1:316:TYR:C     | 2.44                     | 0.42              |
| 4:P1:139:THR:CB    | 8:T1:44:VAL:HB     | 2.49                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Q1:29:SER:CB     | 5:Q1:32:ARG:HD3    | 2.49                     | 0.42              |
| 12:22:80:PHE:HB3   | 26:H2:64:ARG:HH12  | 1.82                     | 0.42              |
| 23:E2:119:CYS:SG   | 23:E2:120:GLU:N    | 2.92                     | 0.42              |
| 52:12:196:ALA:HB2  | 52:12:274:ARG:HH21 | 1.83                     | 0.42              |
| 53:62:88:MET:HE1   | 53:62:468:ILE:HD13 | 2.00                     | 0.42              |
| 55:e2:77:LYS:CG    | 55:e2:78:LEU:H     | 2.32                     | 0.42              |
| 56:A3:106:PRO:HB2  | 56:A3:107:PRO:HD3  | 2.01                     | 0.42              |
| 62:G3:5:LYS:NZ     | 62:G3:6:GLY:N      | 2.54                     | 0.42              |
| 64:I3:26:MET:N     | 64:I3:26:MET:SD    | 2.91                     | 0.42              |
| 1:A1:297:ILE:H     | 1:A1:297:ILE:HG12  | 1.63                     | 0.42              |
| 1:A1:311:ASN:OD1   | 1:A1:320:LEU:HD23  | 2.18                     | 0.42              |
| 1:A1:328:HIS:NE2   | 1:A1:329:MET:HG2   | 2.35                     | 0.42              |
| 2:B1:295:LEU:HD12  | 2:B1:295:LEU:HA    | 1.88                     | 0.42              |
| 3:C1:235:LEU:HG    | 3:C1:236:ILE:N     | 2.32                     | 0.42              |
| 3:C1:257:THR:O     | 3:C1:258:PRO:C     | 2.61                     | 0.42              |
| 1:M1:63:ALA:HB2    | 1:M1:97:TYR:HE2    | 1.84                     | 0.42              |
| 1:M1:85:HIS:CD2    | 2:N1:370:MET:HE1   | 2.54                     | 0.42              |
| 2:N1:279:LEU:HD23  | 2:N1:295:LEU:HD13  | 2.00                     | 0.42              |
| 3:O1:44:GLN:OE1    | 3:O1:44:GLN:HA     | 2.19                     | 0.42              |
| 3:O1:146:ILE:O     | 3:O1:147:THR:C     | 2.62                     | 0.42              |
| 5:Q1:40:THR:HG22   | 10:V1:20:PHE:CZ    | 2.51                     | 0.42              |
| 5:Q1:102:THR:H     | 5:Q1:105:GLU:CB    | 2.32                     | 0.42              |
| 18:92:92:TRP:HB3   | 18:92:127:VAL:HG22 | 2.00                     | 0.42              |
| 19:A2:674:LEU:CD1  | 29:K2:46:LYS:CE    | 2.90                     | 0.42              |
| 22:D2:108:ARG:HD3  | 52:12:36:GLY:HA2   | 2.01                     | 0.42              |
| 34:Q2:30:HIS:CD2   | 34:Q2:120:PRO:HG2  | 2.55                     | 0.42              |
| 34:Q2:137:LEU:HD12 | 34:Q2:138:PRO:HD2  | 2.01                     | 0.42              |
| 46:c2:40:VAL:HA    | 46:c2:41:SER:HA    | 1.63                     | 0.42              |
| 56:A3:474:GLU:HG3  | 56:A3:475:ALA:N    | 2.34                     | 0.42              |
| 57:B3:162:SER:HB3  | 57:B3:197:SER:C    | 2.44                     | 0.42              |
| 58:C3:80:ARG:HG2   | 58:C3:233:PHE:CE1  | 2.54                     | 0.42              |
| 59:D3:37:GLN:O     | 59:D3:41:LYS:HG2   | 2.18                     | 0.42              |
| 60:E3:43:PRO:HB2   | 60:E3:48:ILE:CD1   | 2.48                     | 0.42              |
| 1:A1:61:HIS:HB2    | 1:A1:130:GLU:HG3   | 2.00                     | 0.42              |
| 1:A1:80:GLU:O      | 1:A1:81:SER:C      | 2.63                     | 0.42              |
| 1:A1:381:ARG:O     | 1:A1:382:SER:C     | 2.62                     | 0.42              |
| 3:C1:78:ILE:HG21   | 3:C1:78:ILE:HD13   | 1.80                     | 0.42              |
| 3:C1:235:LEU:HD12  | 3:C1:235:LEU:O     | 2.19                     | 0.42              |
| 3:C1:239:LEU:O     | 3:C1:243:VAL:HB    | 2.19                     | 0.42              |
| 4:D1:43:MET:HA     | 4:D1:112:ASP:OD1   | 2.20                     | 0.42              |
| 6:F1:48:ARG:HD3    | 6:F1:48:ARG:HA     | 1.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F1:88:SER:O      | 6:F1:92:PRO:HD3    | 2.18                     | 0.42              |
| 10:J1:24:ILE:O     | 10:J1:25:VAL:C     | 2.62                     | 0.42              |
| 1:M1:59:VAL:CG2    | 1:M1:186:LEU:HD11  | 2.50                     | 0.42              |
| 2:N1:59:ASN:OD1    | 2:N1:60:SER:N      | 2.43                     | 0.42              |
| 2:N1:90:GLU:O      | 2:N1:91:ALA:C      | 2.62                     | 0.42              |
| 3:O1:183:PHE:CE1   | 3:O1:187:PHE:HE2   | 2.37                     | 0.42              |
| 3:O1:192:ILE:N     | 3:O1:192:ILE:CD1   | 2.82                     | 0.42              |
| 3:O1:235:LEU:O     | 3:O1:235:LEU:HD12  | 2.19                     | 0.42              |
| 3:O1:366:MET:N     | 3:O1:367:PRO:HD2   | 2.33                     | 0.42              |
| 4:P1:116:ILE:O     | 4:P1:117:VAL:C     | 2.60                     | 0.42              |
| 4:P1:149:PHE:CZ    | 8:T1:55:THR:HG23   | 2.53                     | 0.42              |
| 4:P1:192:TRP:CE3   | 4:P1:193:ALA:N     | 2.88                     | 0.42              |
| 5:Q1:114:VAL:HG13  | 5:Q1:120:PRO:HB3   | 2.01                     | 0.42              |
| 5:Q1:134:ILE:HD13  | 5:Q1:134:ILE:HG21  | 1.76                     | 0.42              |
| 5:Q1:172:ARG:HE    | 5:Q1:172:ARG:HB3   | 1.67                     | 0.42              |
| 6:R1:71:ARG:O      | 6:R1:72:GLN:HB2    | 2.19                     | 0.42              |
| 8:T1:67:HIS:O      | 8:T1:68:CYS:C      | 2.63                     | 0.42              |
| 14:42:62:SER:HB2   | 14:42:457:PRO:HD3  | 2.00                     | 0.42              |
| 18:92:195:ASP:OD2  | 18:92:220:SER:OG   | 2.34                     | 0.42              |
| 19:A2:111:LYS:CE   | 33:P2:53:TYR:CE2   | 2.93                     | 0.42              |
| 20:B2:116:LEU:HA   | 22:D2:130:THR:HG21 | 2.02                     | 0.42              |
| 20:B2:193:ASP:O    | 20:B2:194:ILE:C    | 2.61                     | 0.42              |
| 35:R2:200:ILE:O    | 35:R2:262:THR:OG1  | 2.30                     | 0.42              |
| 36:S2:187:LEU:HD13 | 36:S2:277:ARG:HB2  | 2.01                     | 0.42              |
| 48:f2:166:LEU:HA   | 48:f2:167:TRP:HA   | 1.64                     | 0.42              |
| 53:62:492:ILE:HA   | 53:62:495:ILE:HD12 | 2.02                     | 0.42              |
| 56:A3:377:PHE:CD2  | 79:A3:602:HEA:HAD1 | 2.53                     | 0.42              |
| 57:B3:5:MET:CE     | 66:K3:42:PRO:HA    | 2.45                     | 0.42              |
| 1:A1:151:ASN:O     | 1:A1:154:HIS:N     | 2.53                     | 0.42              |
| 1:A1:277:ILE:O     | 1:A1:292:SER:OG    | 2.30                     | 0.42              |
| 2:B1:83:PHE:CE1    | 6:R1:104:ARG:HG2   | 2.54                     | 0.42              |
| 2:B1:92:VAL:O      | 2:B1:92:VAL:CG1    | 2.68                     | 0.42              |
| 2:B1:92:VAL:HG11   | 2:B1:115:ASP:HB3   | 2.02                     | 0.42              |
| 2:B1:206:LEU:HA    | 2:B1:206:LEU:HD12  | 1.85                     | 0.42              |
| 3:C1:248:ASP:CG    | 4:D1:118:ARG:HH21  | 2.28                     | 0.42              |
| 3:C1:372:ILE:HD13  | 3:C1:372:ILE:HG21  | 1.84                     | 0.42              |
| 4:D1:116:ILE:CD1   | 4:D1:120:ARG:HH11  | 2.32                     | 0.42              |
| 4:D1:158:ILE:CG1   | 4:D1:159:GLY:N     | 2.82                     | 0.42              |
| 5:E1:51:ALA:O      | 5:E1:52:LYS:C      | 2.62                     | 0.42              |
| 6:F1:64:ARG:O      | 6:F1:68:LEU:HD12   | 2.20                     | 0.42              |
| 10:J1:43:TYR:O     | 10:J1:43:TYR:CG    | 2.73                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:M1:149:VAL:CG1  | 1:M1:150:PHE:N     | 2.81                     | 0.42              |
| 1:M1:195:MET:HE3  | 1:M1:195:MET:HB3   | 1.61                     | 0.42              |
| 1:M1:334:MET:HA   | 1:M1:334:MET:CE    | 2.49                     | 0.42              |
| 2:N1:72:ALA:HB1   | 2:N1:75:LEU:CD1    | 2.49                     | 0.42              |
| 2:N1:99:THR:OG1   | 9:U1:68:VAL:HG13   | 2.19                     | 0.42              |
| 2:N1:102:ARG:NH1  | 2:N1:174:ASN:O     | 2.53                     | 0.42              |
| 2:N1:312:PHE:CD1  | 9:U1:58:GLN:O      | 2.73                     | 0.42              |
| 3:O1:170:VAL:O    | 3:O1:170:VAL:CG1   | 2.68                     | 0.42              |
| 3:O1:218:ILE:HG22 | 3:O1:223:TYR:HD2   | 1.85                     | 0.42              |
| 4:P1:23:HIS:O     | 4:P1:26:ILE:HB     | 2.20                     | 0.42              |
| 4:P1:178:THR:HG23 | 8:T1:15:ASP:N      | 2.34                     | 0.42              |
| 4:P1:233:ARG:O    | 4:P1:234:LYS:HE2   | 2.19                     | 0.42              |
| 5:Q1:62:MET:HE3   | 5:Q1:62:MET:HB3    | 1.79                     | 0.42              |
| 5:Q1:97:PHE:CD1   | 5:Q1:137:GLY:HA3   | 2.54                     | 0.42              |
| 6:R1:73:GLN:HG2   | 7:S1:36:ASN:ND2    | 2.34                     | 0.42              |
| 6:R1:84:GLU:H     | 6:R1:84:GLU:CD     | 2.28                     | 0.42              |
| 17:82:316:ALA:HB1 | 17:82:326:LEU:HD22 | 2.02                     | 0.42              |
| 19:A2:380:ASP:HB2 | 29:K2:41:TYR:OH    | 2.20                     | 0.42              |
| 23:E2:38:TYR:HB2  | 33:P2:106:LEU:HA   | 2.00                     | 0.42              |
| 30:L2:25:ILE:HB   | 52:12:299:ALA:HB1  | 2.00                     | 0.42              |
| 36:S2:202:VAL:HA  | 36:S2:205:ARG:HB2  | 2.01                     | 0.42              |
| 46:c2:22:TRP:O    | 46:c2:26:GLN:N     | 2.52                     | 0.42              |
| 53:62:358:LYS:HB3 | 53:62:437:PHE:HA   | 2.02                     | 0.42              |
| 60:E3:90:ARG:HD3  | 60:E3:90:ARG:HA    | 1.77                     | 0.42              |
| 66:K3:9:PHE:CD1   | 66:K3:9:PHE:C      | 2.97                     | 0.42              |
| 1:A1:54:GLY:O     | 1:A1:55:ALA:O      | 2.37                     | 0.42              |
| 1:A1:56:GLY:O     | 1:A1:59:VAL:HB     | 2.19                     | 0.42              |
| 1:A1:213:GLN:HB3  | 1:A1:215:HIS:CD2   | 2.53                     | 0.42              |
| 1:A1:436:ARG:NE   | 3:C1:222:PRO:HG3   | 2.33                     | 0.42              |
| 2:B1:158:HIS:ND1  | 2:B1:246:GLU:OE1   | 2.52                     | 0.42              |
| 3:C1:3:ASN:HA     | 3:C1:8:HIS:CD2     | 2.55                     | 0.42              |
| 3:C1:126:THR:HG21 | 69:C1:401:HEM:C3B  | 2.54                     | 0.42              |
| 4:D1:50:HIS:HB3   | 4:D1:54:VAL:HG21   | 2.01                     | 0.42              |
| 10:J1:49:GLY:H    | 10:J1:54:HIS:CD2   | 2.37                     | 0.42              |
| 1:M1:28:GLU:OE1   | 1:M1:375:VAL:CG1   | 2.68                     | 0.42              |
| 1:M1:168:GLU:H    | 1:M1:168:GLU:HG3   | 1.66                     | 0.42              |
| 2:N1:29:LEU:HG    | 2:N1:33:LEU:CD2    | 2.50                     | 0.42              |
| 2:N1:213:HIS:HD2  | 2:N1:213:HIS:O     | 2.02                     | 0.42              |
| 3:O1:244:LEU:O    | 4:P1:201:ARG:HG2   | 2.20                     | 0.42              |
| 4:P1:43:MET:HE3   | 4:P1:91:PHE:CE2    | 2.54                     | 0.42              |
| 4:P1:139:THR:CG2  | 8:T1:44:VAL:HB     | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Q1:129:LYS:HA    | 5:Q1:130:PRO:HD2   | 1.85                     | 0.42              |
| 19:A2:63:PHE:O     | 19:A2:181:ARG:NH2  | 2.51                     | 0.42              |
| 19:A2:359:ASN:HD21 | 29:K2:17:ARG:HG2   | 1.85                     | 0.42              |
| 20:B2:447:VAL:HA   | 20:B2:450:ILE:HD12 | 2.02                     | 0.42              |
| 23:E2:53:VAL:O     | 23:E2:57:ALA:N     | 2.53                     | 0.42              |
| 27:I2:108:LYS:HA   | 27:I2:120:ARG:HA   | 2.01                     | 0.42              |
| 32:O2:77:ARG:HA    | 32:O2:80:ASP:HB3   | 2.01                     | 0.42              |
| 53:62:163:ASP:O    | 53:62:167:ALA:N    | 2.51                     | 0.42              |
| 56:A3:311:ILE:HG21 | 56:A3:311:ILE:HD13 | 1.75                     | 0.42              |
| 58:C3:137:LEU:HA   | 58:C3:137:LEU:HD12 | 1.69                     | 0.42              |
| 58:C3:154:GLY:CA   | 61:F3:6:VAL:HG22   | 2.47                     | 0.42              |
| 63:H3:57:ARG:HA    | 63:H3:60:TYR:CD2   | 2.55                     | 0.42              |
| 3:C1:30:TRP:O      | 3:C1:33:PHE:CD2    | 2.62                     | 0.42              |
| 3:C1:36:LEU:HD22   | 3:C1:235:LEU:HB2   | 2.02                     | 0.42              |
| 3:C1:73:VAL:O      | 3:C1:73:VAL:HG12   | 2.19                     | 0.42              |
| 4:D1:237:TYR:HE2   | 4:D1:239:PRO:HG3   | 1.80                     | 0.42              |
| 6:F1:10:SER:HA     | 6:F1:13:LEU:HG     | 2.01                     | 0.42              |
| 1:M1:88:ALA:O      | 2:N1:286:LYS:HD2   | 2.20                     | 0.42              |
| 1:M1:100:LYS:HG2   | 2:N1:370:MET:SD    | 2.59                     | 0.42              |
| 2:N1:34:VAL:O      | 2:N1:35:ILE:HG22   | 2.19                     | 0.42              |
| 2:N1:156:GLN:OE1   | 9:U1:58:GLN:NE2    | 2.39                     | 0.42              |
| 2:N1:201:SER:OG    | 2:N1:226:ILE:N     | 2.51                     | 0.42              |
| 2:N1:304:HIS:HD2   | 2:N1:306:PRO:CD    | 2.28                     | 0.42              |
| 3:O1:126:THR:CG2   | 69:O1:401:HEM:C3B  | 3.01                     | 0.42              |
| 7:S1:71:ARG:NH2    | 8:T1:60:ASP:OD1    | 2.38                     | 0.42              |
| 19:A2:359:ASN:ND2  | 29:K2:68:ARG:HH22  | 2.17                     | 0.42              |
| 21:C2:116:LEU:HD23 | 21:C2:168:TYR:HB3  | 2.02                     | 0.42              |
| 23:E2:79:ARG:NH2   | 33:P2:19:ASP:OD2   | 2.50                     | 0.42              |
| 28:J2:55:SER:OG    | 28:J2:56:GLY:N     | 2.52                     | 0.42              |
| 53:62:336:LYS:HA   | 53:62:339:LEU:HB3  | 2.01                     | 0.42              |
| 53:62:583:LEU:HD23 | 53:62:586:LEU:HD13 | 2.02                     | 0.42              |
| 79:A3:601:HEA:HHC  | 79:A3:601:HEA:H122 | 2.02                     | 0.42              |
| 1:A1:5:ALA:O       | 1:A1:6:GLN:O       | 2.38                     | 0.42              |
| 1:A1:106:LEU:HA    | 1:A1:106:LEU:HD12  | 1.74                     | 0.42              |
| 1:A1:255:ILE:CD1   | 1:A1:335:MET:HE1   | 2.49                     | 0.42              |
| 1:A1:257:VAL:N     | 1:A1:320:LEU:O     | 2.48                     | 0.42              |
| 1:A1:262:TRP:CE3   | 1:A1:385:THR:CG2   | 3.02                     | 0.42              |
| 1:A1:280:TYR:CD1   | 1:A1:280:TYR:C     | 2.98                     | 0.42              |
| 1:A1:366:VAL:HG11  | 2:B1:44:ALA:HB2    | 2.01                     | 0.42              |
| 2:B1:57:TYR:HB3    | 2:B1:198:HIS:CE1   | 2.55                     | 0.42              |
| 2:B1:72:ALA:HB2    | 2:B1:140:LEU:CD2   | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B1:162:ASN:CB    | 2:B1:244:ILE:HG21  | 2.50                     | 0.42              |
| 2:B1:239:TYR:OH    | 2:B1:423:SER:OG    | 2.37                     | 0.42              |
| 3:C1:177:ARG:O     | 3:C1:181:PHE:CD2   | 2.72                     | 0.42              |
| 3:C1:313:ARG:HH11  | 3:C1:313:ARG:HD2   | 1.59                     | 0.42              |
| 4:D1:7:PRO:HB2     | 4:D1:125:ASP:CB    | 2.49                     | 0.42              |
| 4:D1:69:GLU:O      | 4:D1:73:GLY:CA     | 2.67                     | 0.42              |
| 4:D1:171:PHE:HZ    | 4:D1:182:VAL:HG22  | 1.85                     | 0.42              |
| 4:D1:187:CYS:O     | 4:D1:188:THR:C     | 2.60                     | 0.42              |
| 4:D1:211:MET:HA    | 4:D1:211:MET:CE    | 2.49                     | 0.42              |
| 4:D1:237:TYR:HD1   | 7:G1:13:VAL:HG22   | 1.85                     | 0.42              |
| 1:M1:67:THR:OG1    | 1:M1:119:ASN:HB2   | 2.20                     | 0.42              |
| 1:M1:329:MET:HA    | 1:M1:329:MET:CE    | 2.50                     | 0.42              |
| 2:N1:31:ASN:HB3    | 2:N1:201:SER:CB    | 2.50                     | 0.42              |
| 2:N1:294:SER:O     | 2:N1:297:GLN:N     | 2.53                     | 0.42              |
| 3:O1:234:LEU:O     | 3:O1:237:LEU:HB3   | 2.19                     | 0.42              |
| 3:O1:314:SER:OG    | 3:O1:316:MET:HB3   | 2.19                     | 0.42              |
| 4:P1:58:GLU:O      | 4:P1:62:LYS:HB2    | 2.19                     | 0.42              |
| 4:P1:206:LEU:O     | 4:P1:207:LYS:C     | 2.61                     | 0.42              |
| 4:P1:240:PRO:CG    | 4:P1:241:LYS:H     | 2.33                     | 0.42              |
| 6:R1:67:ASP:HA     | 6:R1:70:MET:HE3    | 2.01                     | 0.42              |
| 17:82:297:LYS:N    | 17:82:333:GLU:O    | 2.45                     | 0.42              |
| 19:A2:34:VAL:HG13  | 19:A2:100:TRP:H    | 1.84                     | 0.42              |
| 19:A2:140:GLN:NE2  | 20:B2:382:PHE:CD2  | 2.88                     | 0.42              |
| 19:A2:583:ILE:CD1  | 38:U2:137:TRP:HZ3  | 2.31                     | 0.42              |
| 23:E2:211:TYR:CZ   | 33:P2:39:PRO:HG3   | 2.55                     | 0.42              |
| 29:K2:55:ILE:O     | 29:K2:56:ARG:NH1   | 2.43                     | 0.42              |
| 35:R2:266:VAL:HG23 | 35:R2:335:LEU:HB3  | 2.02                     | 0.42              |
| 36:S2:187:LEU:HA   | 36:S2:188:PRO:HD3  | 1.84                     | 0.42              |
| 43:Z2:24:ILE:HG23  | 43:Z2:54:MET:HE1   | 2.02                     | 0.42              |
| 53:62:439:THR:OG1  | 53:62:440:LEU:N    | 2.42                     | 0.42              |
| 56:A3:247:ILE:HB   | 79:A3:602:HEA:HBC1 | 2.01                     | 0.42              |
| 1:A1:38:GLY:HA3    | 1:A1:40:TRP:CZ3    | 2.50                     | 0.42              |
| 1:A1:64:PHE:CE1    | 1:A1:86:LEU:CG     | 2.81                     | 0.42              |
| 1:A1:361:LEU:HD12  | 1:A1:361:LEU:O     | 2.19                     | 0.42              |
| 2:B1:81:SER:O      | 2:B1:82:SER:C      | 2.62                     | 0.42              |
| 2:B1:129:ALA:O     | 2:B1:130:PRO:C     | 2.62                     | 0.42              |
| 2:B1:312:PHE:N     | 2:B1:323:GLY:O     | 2.47                     | 0.42              |
| 3:C1:172:LYS:O     | 3:C1:173:ALA:C     | 2.60                     | 0.42              |
| 4:D1:8:PRO:O       | 4:D1:125:ASP:CG    | 2.63                     | 0.42              |
| 4:D1:57:THR:CG2    | 4:D1:58:GLU:N      | 2.83                     | 0.42              |
| 4:D1:223:LYS:NZ    | 4:D1:227:TRP:CD1   | 2.86                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F1:94:LEU:O      | 6:F1:94:LEU:HD12   | 2.20                     | 0.42              |
| 10:J1:3:PRO:O      | 10:J1:4:THR:C      | 2.63                     | 0.42              |
| 1:M1:158:PHE:HB2   | 1:M1:164:ALA:HB2   | 2.02                     | 0.42              |
| 1:M1:213:GLN:HB2   | 1:M1:215:HIS:CD2   | 2.55                     | 0.42              |
| 1:M1:345:LEU:HA    | 1:M1:345:LEU:HD23  | 1.69                     | 0.42              |
| 1:M1:420:PRO:HG3   | 1:M1:441:MET:SD    | 2.60                     | 0.42              |
| 1:M1:428:ILE:CG2   | 1:M1:431:LEU:CG    | 2.97                     | 0.42              |
| 3:O1:14:VAL:O      | 3:O1:14:VAL:HG12   | 2.20                     | 0.42              |
| 3:O1:41:LEU:HD12   | 69:O1:401:HEM:HBB1 | 2.00                     | 0.42              |
| 5:Q1:13:TYR:O      | 7:S1:24:ARG:HG3    | 2.20                     | 0.42              |
| 12:22:7:ILE:O      | 12:22:11:LEU:N     | 2.53                     | 0.42              |
| 15:52:32:CYS:O     | 15:52:36:MET:N     | 2.53                     | 0.42              |
| 74:82:501:FMN:O4'  | 74:82:501:FMN:O2'  | 2.34                     | 0.42              |
| 19:A2:511:LYS:HD3  | 19:A2:663:ASN:HB3  | 2.02                     | 0.42              |
| 19:A2:613:PRO:CG   | 38:U2:134:ILE:HG21 | 2.46                     | 0.42              |
| 52:12:75:PRO:CB    | 52:12:223:PHE:CZ   | 2.99                     | 0.42              |
| 52:12:126:LYS:CD   | 52:12:126:LYS:C    | 2.89                     | 0.42              |
| 56:A3:356:ILE:HD13 | 56:A3:356:ILE:HA   | 1.90                     | 0.42              |
| 59:D3:126:MET:HG3  | 59:D3:128:VAL:HG23 | 2.00                     | 0.42              |
| 60:E3:93:LEU:HD23  | 60:E3:93:LEU:HA    | 1.88                     | 0.42              |
| 1:A1:43:ALA:CB     | 1:A1:189:HIS:CB    | 2.97                     | 0.42              |
| 2:B1:283:PRO:CG    | 9:I1:55:LEU:HD13   | 2.50                     | 0.42              |
| 3:C1:53:MET:SD     | 3:O1:181:PHE:HZ    | 2.43                     | 0.42              |
| 3:C1:159:ASN:O     | 3:C1:162:GLU:HB2   | 2.20                     | 0.42              |
| 3:C1:184:ILE:O     | 3:C1:184:ILE:HG12  | 2.19                     | 0.42              |
| 3:C1:317:PHE:CD1   | 6:F1:26:PHE:HB3    | 2.55                     | 0.42              |
| 3:C1:365:LEU:O     | 3:C1:366:MET:C     | 2.61                     | 0.42              |
| 3:C1:373:GLU:O     | 3:C1:377:LEU:HD12  | 2.19                     | 0.42              |
| 4:D1:44:ASP:OD1    | 4:D1:93:LYS:HE3    | 2.20                     | 0.42              |
| 4:D1:57:THR:CG2    | 4:D1:58:GLU:H      | 2.32                     | 0.42              |
| 4:D1:146:GLY:O     | 4:D1:148:TYR:CD1   | 2.73                     | 0.42              |
| 4:D1:162:PRO:O     | 4:D1:163:PRO:C     | 2.63                     | 0.42              |
| 11:K1:20:THR:HG23  | 11:K1:24:TRP:HD1   | 1.83                     | 0.42              |
| 1:M1:152:TYR:CE2   | 1:M1:243:HIS:HD2   | 2.38                     | 0.42              |
| 2:N1:81:SER:O      | 2:N1:82:SER:C      | 2.63                     | 0.42              |
| 2:N1:343:GLN:O     | 2:N1:343:GLN:HG3   | 2.20                     | 0.42              |
| 3:O1:233:LEU:HD12  | 3:O1:233:LEU:HA    | 1.74                     | 0.42              |
| 4:P1:115:TYR:O     | 4:P1:116:ILE:C     | 2.60                     | 0.42              |
| 9:U1:66:ALA:O      | 9:U1:77:ARG:HG3    | 2.20                     | 0.42              |
| 11:W1:20:THR:HG23  | 11:W1:24:TRP:HD1   | 1.85                     | 0.42              |
| 35:R2:320:GLU:O    | 35:R2:324:THR:OG1  | 2.38                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:S2:135:LEU:HA   | 36:S2:138:LEU:HD13 | 2.02                     | 0.42              |
| 45:b2:96:ALA:HA    | 45:b2:97:GLU:HA    | 1.67                     | 0.42              |
| 55:e2:75:TYR:H     | 55:e2:75:TYR:HD2   | 1.68                     | 0.42              |
| 58:C3:224:LYS:NZ   | 58:C3:226:HIS:HE2  | 2.18                     | 0.42              |
| 59:D3:86:MET:O     | 66:K3:25:CYS:HB2   | 2.20                     | 0.42              |
| 61:F3:86:GLY:O     | 61:F3:87:THR:O     | 2.37                     | 0.42              |
| 64:I3:35:TYR:O     | 64:I3:39:VAL:HB    | 2.19                     | 0.42              |
| 68:M3:19:LEU:HD23  | 68:M3:19:LEU:C     | 2.45                     | 0.42              |
| 1:A1:253:VAL:O     | 1:A1:323:HIS:HA    | 2.20                     | 0.41              |
| 1:A1:292:SER:O     | 1:A1:293:PRO:C     | 2.63                     | 0.41              |
| 2:B1:168:TYR:CB    | 2:B1:173:ALA:HB2   | 2.44                     | 0.41              |
| 2:B1:282:GLY:HA2   | 2:B1:283:PRO:HD2   | 1.77                     | 0.41              |
| 3:C1:234:LEU:HD21  | 4:D1:216:LEU:HD21  | 2.01                     | 0.41              |
| 4:D1:29:GLY:HA2    | 4:D1:32:VAL:HG23   | 2.02                     | 0.41              |
| 4:D1:150:ASN:OD1   | 4:D1:150:ASN:C     | 2.59                     | 0.41              |
| 10:J1:20:PHE:O     | 10:J1:23:THR:HB    | 2.20                     | 0.41              |
| 1:M1:69:ASN:C      | 1:M1:71:PRO:HD3    | 2.45                     | 0.41              |
| 1:M1:78:GLU:HG2    | 1:M1:112:LEU:HD21  | 2.01                     | 0.41              |
| 1:M1:91:THR:HG22   | 1:M1:94:HIS:N      | 2.33                     | 0.41              |
| 1:M1:137:GLU:O     | 1:M1:138:LEU:C     | 2.63                     | 0.41              |
| 2:N1:180:ASP:HA    | 2:N1:183:ILE:HD12  | 2.02                     | 0.41              |
| 2:N1:243:GLU:HA    | 2:N1:424:MET:O     | 2.20                     | 0.41              |
| 3:O1:15:ASN:ND2    | 3:O1:18:PHE:CD2    | 2.88                     | 0.41              |
| 3:O1:123:VAL:O     | 3:O1:123:VAL:CG1   | 2.65                     | 0.41              |
| 4:P1:10:TYR:CE1    | 4:P1:128:PHE:HE2   | 2.36                     | 0.41              |
| 4:P1:25:SER:O      | 4:P1:26:ILE:C      | 2.61                     | 0.41              |
| 4:P1:164:ILE:CD1   | 4:P1:186:VAL:HG21  | 2.50                     | 0.41              |
| 4:P1:206:LEU:HG    | 4:P1:210:LEU:HD11  | 2.02                     | 0.41              |
| 10:V1:31:PHE:CD2   | 10:V1:31:PHE:C     | 2.98                     | 0.41              |
| 14:42:45:PHE:HA    | 14:42:46:GLY:HA3   | 1.68                     | 0.41              |
| 20:B2:194:ILE:HD13 | 20:B2:268:TRP:HE1  | 1.85                     | 0.41              |
| 37:T2:77:SER:HA    | 37:T2:80:VAL:HG22  | 2.02                     | 0.41              |
| 56:A3:314:ILE:HB   | 56:A3:315:PRO:CD   | 2.51                     | 0.41              |
| 57:B3:100:MET:HE3  | 57:B3:157:GLU:HG3  | 2.02                     | 0.41              |
| 58:C3:252:LEU:HD23 | 58:C3:252:LEU:HA   | 1.90                     | 0.41              |
| 1:A1:33:PRO:O      | 1:A1:103:SER:CB    | 2.67                     | 0.41              |
| 1:A1:46:ARG:NH2    | 1:A1:316:ASP:OD1   | 2.52                     | 0.41              |
| 2:B1:342:ASN:O     | 2:B1:345:LYS:N     | 2.52                     | 0.41              |
| 3:C1:101:GLY:HA2   | 3:C1:106:SER:HB2   | 2.02                     | 0.41              |
| 3:C1:198:LEU:HD22  | 3:O1:11:MET:HG2    | 2.02                     | 0.41              |
| 3:C1:264:THR:HG21  | 5:Q1:144:CYS:SG    | 2.60                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D1:106:ASN:C     | 4:D1:106:ASN:HD22  | 2.28                     | 0.41              |
| 4:D1:204:MET:O     | 4:D1:207:LYS:N     | 2.53                     | 0.41              |
| 2:N1:135:TRP:NE1   | 2:N1:136:GLU:HG3   | 2.35                     | 0.41              |
| 3:O1:211:ILE:CG2   | 6:R1:62:ILE:HD13   | 2.50                     | 0.41              |
| 3:O1:378:LYS:CD    | 6:R1:33:ARG:HH12   | 2.32                     | 0.41              |
| 5:Q1:109:GLU:OE2   | 5:Q1:166:ASP:CG    | 2.63                     | 0.41              |
| 5:Q1:109:GLU:OE2   | 5:Q1:166:ASP:OD2   | 2.37                     | 0.41              |
| 7:S1:33:GLY:O      | 7:S1:37:VAL:HB     | 2.19                     | 0.41              |
| 17:82:383:THR:HG23 | 19:A2:75:CYS:CA    | 2.32                     | 0.41              |
| 18:92:134:VAL:HG23 | 18:92:171:LEU:HD11 | 2.01                     | 0.41              |
| 19:A2:598:ASN:OD1  | 19:A2:601:GLY:N    | 2.53                     | 0.41              |
| 21:C2:230:GLN:HE21 | 21:C2:233:ARG:NH1  | 2.16                     | 0.41              |
| 22:D2:114:ARG:HD2  | 22:D2:114:ARG:O    | 2.20                     | 0.41              |
| 35:R2:154:GLN:HG3  | 35:R2:155:VAL:HG23 | 2.02                     | 0.41              |
| 48:f2:162:ASP:HA   | 48:f2:163:LEU:HA   | 1.79                     | 0.41              |
| 56:A3:354:THR:HG21 | 56:A3:376:HIS:HA   | 2.03                     | 0.41              |
| 58:C3:146:TRP:CE2  | 62:G3:17:ARG:HB2   | 2.56                     | 0.41              |
| 58:C3:146:TRP:NE1  | 62:G3:17:ARG:HB2   | 2.35                     | 0.41              |
| 62:G3:77:PRO:HA    | 62:G3:82:TYR:HA    | 2.02                     | 0.41              |
| 1:A1:136:GLN:NE2   | 9:I1:50:LEU:HG     | 2.35                     | 0.41              |
| 2:B1:24:LEU:CG     | 2:B1:38:LEU:HD11   | 2.31                     | 0.41              |
| 2:B1:134:ARG:HG2   | 2:B1:135:TRP:N     | 2.35                     | 0.41              |
| 2:B1:154:ASN:O     | 2:B1:157:ALA:N     | 2.54                     | 0.41              |
| 4:D1:161:ALA:O     | 4:D1:162:PRO:C     | 2.63                     | 0.41              |
| 1:M1:347:THR:HA    | 11:W1:16:ASN:HD22  | 1.85                     | 0.41              |
| 1:M1:426:GLY:H     | 1:M1:428:ILE:HG13  | 1.83                     | 0.41              |
| 2:N1:56:ARG:HH21   | 2:N1:103:GLU:CD    | 2.29                     | 0.41              |
| 2:N1:200:THR:OG1   | 2:N1:201:SER:N     | 2.53                     | 0.41              |
| 2:N1:255:ALA:HA    | 2:N1:426:ALA:HA    | 2.02                     | 0.41              |
| 2:N1:264:ILE:HD12  | 2:N1:315:SER:OG    | 2.20                     | 0.41              |
| 2:N1:285:VAL:HG12  | 2:N1:285:VAL:O     | 2.20                     | 0.41              |
| 2:N1:309:VAL:CG2   | 2:N1:326:THR:HG22  | 2.50                     | 0.41              |
| 3:O1:10:LEU:HD12   | 3:O1:13:ILE:CD1    | 2.50                     | 0.41              |
| 3:O1:122:THR:HB    | 3:O1:189:ILE:CD1   | 2.49                     | 0.41              |
| 3:O1:156:ILE:O     | 3:O1:158:THR:N     | 2.54                     | 0.41              |
| 4:P1:139:THR:O     | 8:T1:44:VAL:HG11   | 2.20                     | 0.41              |
| 5:Q1:75:GLU:O      | 5:Q1:194:ILE:CA    | 2.47                     | 0.41              |
| 5:Q1:150:ALA:CB    | 5:Q1:157:TYR:CB    | 2.98                     | 0.41              |
| 5:Q1:181:GLU:HG2   | 5:Q1:182:VAL:N     | 2.35                     | 0.41              |
| 5:Q1:184:SER:O     | 5:Q1:195:VAL:HA    | 2.20                     | 0.41              |
| 8:T1:15:ASP:CB     | 8:T1:16:PRO:HD3    | 2.49                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:T1:65:ARG:HH11   | 8:T1:65:ARG:HD2    | 1.65                     | 0.41              |
| 12:22:106:LEU:HD13 | 12:22:139:MET:HE2  | 2.02                     | 0.41              |
| 12:22:108:MET:HE1  | 12:22:191:THR:HG21 | 2.02                     | 0.41              |
| 12:22:216:PHE:HA   | 12:22:219:PHE:HB2  | 2.02                     | 0.41              |
| 19:A2:613:PRO:HB2  | 38:U2:134:ILE:HD12 | 2.01                     | 0.41              |
| 20:B2:238:LEU:HD13 | 33:P2:37:PRO:HD2   | 2.02                     | 0.41              |
| 22:D2:150:VAL:HB   | 22:D2:179:VAL:HA   | 2.02                     | 0.41              |
| 23:E2:98:ARG:NH2   | 23:E2:155:CYS:O    | 2.53                     | 0.41              |
| 28:J2:38:VAL:O     | 28:J2:44:GLN:NE2   | 2.53                     | 0.41              |
| 56:A3:461:SER:O    | 56:A3:465:VAL:HG13 | 2.21                     | 0.41              |
| 1:A1:53:ASN:CG     | 1:A1:170:PRO:HD3   | 2.45                     | 0.41              |
| 1:A1:66:GLY:O      | 1:A1:121:SER:N     | 2.50                     | 0.41              |
| 2:B1:55:SER:OG     | 2:B1:102:ARG:HA    | 2.20                     | 0.41              |
| 2:B1:160:ILE:HA    | 2:B1:160:ILE:HD12  | 1.73                     | 0.41              |
| 2:B1:279:LEU:CD2   | 2:B1:344:VAL:HG22  | 2.50                     | 0.41              |
| 3:C1:61:THR:O      | 3:C1:62:ALA:C      | 2.63                     | 0.41              |
| 3:C1:280:ILE:HA    | 3:C1:355:SER:OG    | 2.20                     | 0.41              |
| 3:C1:319:PRO:O     | 3:C1:322:GLN:N     | 2.52                     | 0.41              |
| 4:D1:7:PRO:CG      | 4:D1:126:TYR:HA    | 2.47                     | 0.41              |
| 4:D1:165:TYR:O     | 4:D1:166:ASN:C     | 2.61                     | 0.41              |
| 4:D1:208:MET:HE2   | 4:D1:208:MET:C     | 2.44                     | 0.41              |
| 8:H1:15:ASP:CB     | 8:H1:16:PRO:CD     | 2.97                     | 0.41              |
| 1:M1:31:SER:N      | 1:M1:202:GLY:HA2   | 2.35                     | 0.41              |
| 1:M1:34:THR:OG1    | 2:N1:373:GLU:OE1   | 2.37                     | 0.41              |
| 1:M1:156:THR:OG1   | 1:M1:241:ILE:HB    | 2.21                     | 0.41              |
| 1:M1:166:SER:HB2   | 5:Q1:3:THR:HG22    | 2.02                     | 0.41              |
| 1:M1:236:PHE:HD2   | 1:M1:258:GLU:CB    | 2.29                     | 0.41              |
| 1:M1:369:LEU:HD21  | 1:M1:378:ASP:OD2   | 2.20                     | 0.41              |
| 1:M1:385:THR:HG22  | 1:M1:386:TYR:CD1   | 2.55                     | 0.41              |
| 2:N1:95:LYS:HG3    | 9:U1:70:LEU:HD13   | 2.02                     | 0.41              |
| 2:N1:168:TYR:CZ    | 2:N1:172:LEU:HD12  | 2.56                     | 0.41              |
| 2:N1:435:PHE:N     | 2:N1:438:GLU:HB2   | 2.35                     | 0.41              |
| 3:O1:26:ASN:ND2    | 3:O1:26:ASN:C      | 2.78                     | 0.41              |
| 3:O1:26:ASN:O      | 3:O1:26:ASN:CG     | 2.63                     | 0.41              |
| 3:O1:45:ILE:CD1    | 3:O1:190:MET:HE2   | 2.51                     | 0.41              |
| 3:O1:47:THR:HG23   | 3:O1:79:ILE:HG23   | 2.01                     | 0.41              |
| 3:O1:58:ASP:O      | 3:O1:59:THR:C      | 2.60                     | 0.41              |
| 3:O1:115:ILE:N     | 3:O1:115:ILE:CD1   | 2.83                     | 0.41              |
| 3:O1:219:PRO:HB2   | 3:O1:222:PRO:CD    | 2.50                     | 0.41              |
| 3:O1:282:ARG:NH1   | 3:O1:343:VAL:HG22  | 2.36                     | 0.41              |
| 4:P1:174:GLY:O     | 4:P1:175:THR:C     | 2.61                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:P1:230:LEU:O     | 4:P1:233:ARG:HB2  | 2.19                     | 0.41              |
| 4:P1:240:PRO:HG2   | 4:P1:241:LYS:N    | 2.34                     | 0.41              |
| 5:Q1:41:ALA:HA     | 10:V1:24:ILE:HD11 | 2.03                     | 0.41              |
| 5:Q1:107:ASP:O     | 5:Q1:110:ALA:N    | 2.51                     | 0.41              |
| 5:Q1:119:ASP:OD1   | 5:Q1:120:PRO:CD   | 2.67                     | 0.41              |
| 5:Q1:177:PRO:HB2   | 5:Q1:178:LEU:HG   | 2.03                     | 0.41              |
| 6:R1:74:ILE:HG23   | 6:R1:75:LEU:O     | 2.21                     | 0.41              |
| 15:52:7:ASN:HA     | 15:52:8:ILE:HA    | 1.72                     | 0.41              |
| 20:B2:318:VAL:HA   | 20:B2:319:PRO:HD3 | 1.94                     | 0.41              |
| 24:F2:85:PHE:O     | 24:F2:89:ASN:N    | 2.44                     | 0.41              |
| 39:V2:143:TYR:HD1  | 39:V2:143:TYR:HA  | 1.73                     | 0.41              |
| 60:E3:21:LYS:O     | 60:E3:57:ARG:NH1  | 2.53                     | 0.41              |
| 65:J3:12:PHE:O     | 65:J3:23:LYS:HE2  | 2.21                     | 0.41              |
| 1:A1:134:ILE:O     | 1:A1:137:GLU:N    | 2.53                     | 0.41              |
| 1:A1:143:THR:CG2   | 9:I1:48:SER:H     | 2.18                     | 0.41              |
| 1:A1:280:TYR:HB3   | 1:A1:307:PHE:CD2  | 2.55                     | 0.41              |
| 1:A1:291:SER:OG    | 2:B1:90:GLU:OE1   | 2.26                     | 0.41              |
| 1:A1:426:GLY:H     | 1:A1:428:ILE:HD11 | 1.83                     | 0.41              |
| 2:B1:283:PRO:HG3   | 9:I1:55:LEU:CG    | 2.50                     | 0.41              |
| 3:C1:360:LEU:HA    | 3:C1:360:LEU:HD12 | 1.82                     | 0.41              |
| 4:D1:91:PHE:N      | 4:D1:91:PHE:CD1   | 2.89                     | 0.41              |
| 4:D1:165:TYR:CE1   | 4:D1:168:VAL:HA   | 2.56                     | 0.41              |
| 6:F1:51:PRO:O      | 6:F1:52:GLU:C     | 2.63                     | 0.41              |
| 1:M1:43:ALA:HB1    | 1:M1:189:HIS:CB   | 2.50                     | 0.41              |
| 2:N1:182:ARG:O     | 2:N1:185:LYS:N    | 2.54                     | 0.41              |
| 2:N1:333:ALA:O     | 2:N1:337:ILE:HD12 | 2.20                     | 0.41              |
| 3:O1:277:ALA:HB1   | 3:O1:294:LEU:CD1  | 2.50                     | 0.41              |
| 3:O1:282:ARG:CZ    | 3:O1:343:VAL:HG22 | 2.49                     | 0.41              |
| 3:O1:337:TRP:NE1   | 3:O1:341:GLN:OE1  | 2.54                     | 0.41              |
| 4:P1:102:ARG:HG2   | 4:P1:109:LEU:HB2  | 2.02                     | 0.41              |
| 4:P1:165:TYR:CE2   | 4:P1:168:VAL:HG22 | 2.55                     | 0.41              |
| 4:P1:211:MET:O     | 4:P1:212:MET:C    | 2.62                     | 0.41              |
| 70:P1:301:HEC:CHD  | 70:P1:301:HEC:CBC | 2.95                     | 0.41              |
| 5:Q1:33:LYS:HA     | 7:S1:21:PHE:CE1   | 2.55                     | 0.41              |
| 6:R1:74:ILE:H      | 7:S1:39:ARG:NH2   | 2.19                     | 0.41              |
| 17:82:418:GLN:HE21 | 19:A2:115:GLY:HA3 | 1.70                     | 0.41              |
| 18:92:147:SER:HB2  | 18:92:198:PRO:HG3 | 2.01                     | 0.41              |
| 19:A2:627:SER:OG   | 19:A2:632:MET:O   | 2.31                     | 0.41              |
| 23:E2:85:ASN:O     | 23:E2:89:GLU:N    | 2.42                     | 0.41              |
| 23:E2:114:ILE:HD12 | 23:E2:114:ILE:HA  | 1.97                     | 0.41              |
| 31:N2:26:ILE:O     | 31:N2:30:LYS:N    | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:V2:43:LEU:HB2  | 52:12:179:TRP:HE1 | 1.86                     | 0.41              |
| 42:Y2:89:TYR:O    | 42:Y2:91:ASP:N    | 2.53                     | 0.41              |
| 47:d2:34:ARG:HA   | 47:d2:35:LYS:HA   | 1.70                     | 0.41              |
| 56:A3:198:SER:HB2 | 56:A3:238:PHE:HA  | 2.03                     | 0.41              |
| 56:A3:264:LYS:NZ  | 57:B3:56:MET:HE2  | 2.35                     | 0.41              |
| 58:C3:182:TYR:O   | 62:G3:72:ASN:HB2  | 2.21                     | 0.41              |
| 59:D3:130:PRO:O   | 59:D3:136:ALA:HB2 | 2.20                     | 0.41              |
| 63:H3:24:ASN:HD22 | 63:H3:25:GLN:N    | 2.18                     | 0.41              |
| 1:A1:260:PRO:HG3  | 1:A1:414:TYR:CE1  | 2.55                     | 0.41              |
| 1:A1:314:TYR:HB2  | 1:A1:317:THR:O    | 2.20                     | 0.41              |
| 2:B1:68:LEU:HB2   | 2:B1:144:LEU:HD21 | 2.02                     | 0.41              |
| 2:B1:68:LEU:O     | 2:B1:71:LEU:N     | 2.50                     | 0.41              |
| 2:B1:170:ASN:OD1  | 2:B1:171:ALA:N    | 2.52                     | 0.41              |
| 2:B1:397:THR:O    | 2:B1:398:VAL:C    | 2.63                     | 0.41              |
| 3:C1:163:TRP:CD1  | 5:Q1:63:SER:HA    | 2.55                     | 0.41              |
| 6:F1:28:LYS:HB3   | 6:F1:74:ILE:CD1   | 2.44                     | 0.41              |
| 10:J1:29:LEU:HD12 | 10:J1:32:GLU:OE2  | 2.21                     | 0.41              |
| 11:K1:24:TRP:CE3  | 11:K1:24:TRP:HA   | 2.56                     | 0.41              |
| 1:M1:61:HIS:HB2   | 1:M1:130:GLU:HG3  | 2.02                     | 0.41              |
| 1:M1:64:PHE:HE2   | 1:M1:88:ALA:CB    | 2.34                     | 0.41              |
| 2:N1:33:LEU:HB2   | 2:N1:204:MET:O    | 2.20                     | 0.41              |
| 2:N1:49:LEU:HD21  | 2:N1:204:MET:SD   | 2.60                     | 0.41              |
| 2:N1:160:ILE:CD1  | 2:N1:325:TYR:HE2  | 2.33                     | 0.41              |
| 2:N1:309:VAL:CG1  | 2:N1:310:SER:N    | 2.82                     | 0.41              |
| 2:N1:436:ILE:H    | 2:N1:436:ILE:HG13 | 1.41                     | 0.41              |
| 3:O1:11:MET:O     | 3:O1:14:VAL:HB    | 2.21                     | 0.41              |
| 3:O1:196:HIS:HE1  | 69:O1:402:HEM:CHD | 2.32                     | 0.41              |
| 3:O1:211:ILE:CG2  | 3:O1:212:SER:N    | 2.83                     | 0.41              |
| 3:O1:276:PHE:CE2  | 3:O1:297:SER:OG   | 2.74                     | 0.41              |
| 3:O1:284:ILE:HG23 | 3:O1:285:PRO:HD2  | 2.02                     | 0.41              |
| 4:P1:120:ARG:HD2  | 70:P1:301:HEC:CGA | 2.50                     | 0.41              |
| 4:P1:138:PRO:CG   | 8:T1:55:THR:HA    | 2.50                     | 0.41              |
| 5:Q1:31:ALA:HB2   | 10:V1:7:ALA:HB2   | 2.03                     | 0.41              |
| 6:R1:35:ASP:OD2   | 6:R1:61:ARG:HD2   | 2.20                     | 0.41              |
| 10:V1:52:TRP:N    | 10:V1:52:TRP:HE3  | 2.18                     | 0.41              |
| 17:82:36:LYS:HB2  | 17:82:38:GLU:HG3  | 2.01                     | 0.41              |
| 19:A2:613:PRO:HG3 | 38:U2:134:ILE:CG2 | 2.51                     | 0.41              |
| 23:E2:54:THR:HG22 | 30:L2:13:TRP:HH2  | 1.85                     | 0.41              |
| 27:I2:87:CYS:O    | 27:I2:96:HIS:NE2  | 2.53                     | 0.41              |
| 28:J2:41:TYR:OH   | 52:12:317:GLN:NE2 | 2.39                     | 0.41              |
| 51:j2:21:LEU:HD11 | 51:j2:81:TYR:HB2  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:B3:146:MET:SD   | 57:B3:189:PRO:HB3  | 2.60                     | 0.41              |
| 58:C3:6:HIS:CD2    | 58:C3:8:TYR:HB2    | 2.55                     | 0.41              |
| 59:D3:11:TYR:CD1   | 59:D3:11:TYR:C     | 2.99                     | 0.41              |
| 1:A1:4:TYR:O       | 1:A1:5:ALA:C       | 2.63                     | 0.41              |
| 1:A1:433:ASP:O     | 1:A1:436:ARG:N     | 2.52                     | 0.41              |
| 2:B1:211:VAL:HG11  | 2:B1:216:LEU:HD13  | 2.02                     | 0.41              |
| 2:B1:250:ASP:OD1   | 2:B1:251:SER:N     | 2.54                     | 0.41              |
| 3:C1:122:THR:HG21  | 3:C1:189:ILE:HG12  | 2.03                     | 0.41              |
| 4:D1:55:CYS:SG     | 10:J1:52:TRP:HB2   | 2.60                     | 0.41              |
| 6:F1:68:LEU:HD11   | 6:F1:75:LEU:HD13   | 2.01                     | 0.41              |
| 7:G1:31:SER:O      | 7:G1:35:PRO:CD     | 2.62                     | 0.41              |
| 8:H1:59:LEU:HD23   | 8:H1:59:LEU:HA     | 1.76                     | 0.41              |
| 8:H1:61:PHE:O      | 8:H1:62:LEU:C      | 2.64                     | 0.41              |
| 1:M1:48:GLU:HB3    | 1:M1:52:ASN:O      | 2.21                     | 0.41              |
| 1:M1:257:VAL:O     | 1:M1:320:LEU:HB2   | 2.21                     | 0.41              |
| 1:M1:282:CYS:SG    | 1:M1:305:GLN:CD    | 3.03                     | 0.41              |
| 1:M1:426:GLY:H     | 1:M1:428:ILE:CG1   | 2.30                     | 0.41              |
| 2:N1:47:ILE:HB     | 2:N1:109:VAL:HG12  | 2.02                     | 0.41              |
| 2:N1:346:THR:O     | 2:N1:347:ILE:C     | 2.62                     | 0.41              |
| 3:O1:88:SER:HA     | 3:O1:272:TRP:CZ2   | 2.53                     | 0.41              |
| 3:O1:133:LEU:HA    | 3:O1:175:LEU:HD11  | 2.01                     | 0.41              |
| 3:O1:149:LEU:O     | 3:O1:291:VAL:HG21  | 2.21                     | 0.41              |
| 3:O1:184:ILE:O     | 3:O1:184:ILE:HG12  | 2.20                     | 0.41              |
| 4:P1:48:TYR:OH     | 4:P1:68:VAL:HG21   | 2.21                     | 0.41              |
| 4:P1:153:PHE:O     | 4:P1:154:PRO:C     | 2.64                     | 0.41              |
| 4:P1:224:ARG:O     | 4:P1:225:HIS:C     | 2.62                     | 0.41              |
| 5:Q1:87:MET:O      | 5:Q1:89:PHE:HD1    | 2.04                     | 0.41              |
| 5:Q1:185:TYR:HD2   | 5:Q1:193:VAL:HG21  | 1.84                     | 0.41              |
| 6:R1:55:TYR:CD1    | 6:R1:55:TYR:C      | 2.99                     | 0.41              |
| 11:W1:24:TRP:HA    | 11:W1:24:TRP:CE3   | 2.55                     | 0.41              |
| 12:22:190:MET:HB2  | 12:22:201:THR:HG23 | 2.02                     | 0.41              |
| 13:32:84:LEU:HD21  | 52:12:309:ILE:HD13 | 2.03                     | 0.41              |
| 16:72:140:ALA:HA   | 16:72:142:GLY:N    | 2.36                     | 0.41              |
| 18:92:93:LEU:HA    | 18:92:94:PRO:HD3   | 1.94                     | 0.41              |
| 19:A2:44:GLU:HB3   | 19:A2:47:THR:HG23  | 2.03                     | 0.41              |
| 23:E2:135:ARG:NH1  | 27:I2:68:ALA:O     | 2.54                     | 0.41              |
| 35:R2:126:VAL:HG13 | 35:R2:164:PHE:HD1  | 1.86                     | 0.41              |
| 35:R2:227:PRO:HG2  | 35:R2:230:SER:HA   | 2.02                     | 0.41              |
| 56:A3:23:GLY:HA3   | 56:A3:73:ILE:HG13  | 2.03                     | 0.41              |
| 56:A3:462:LEU:O    | 56:A3:466:MET:HG3  | 2.20                     | 0.41              |
| 56:A3:501:PRO:O    | 56:A3:502:TYR:C    | 2.63                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:B3:193:TYR:CD1  | 57:B3:193:TYR:N    | 2.88                     | 0.41              |
| 1:A1:8:LEU:HD23    | 1:A1:8:LEU:HA      | 1.94                     | 0.41              |
| 1:A1:29:GLN:HG3    | 1:A1:203:LEU:O     | 2.21                     | 0.41              |
| 1:A1:97:TYR:CD1    | 1:A1:97:TYR:N      | 2.88                     | 0.41              |
| 1:A1:244:ARG:NH1   | 7:G1:10:VAL:HG21   | 2.35                     | 0.41              |
| 1:A1:292:SER:HA    | 1:A1:293:PRO:HD2   | 1.88                     | 0.41              |
| 1:A1:385:THR:HB    | 1:A1:386:TYR:HD1   | 1.83                     | 0.41              |
| 3:C1:200:LEU:CD1   | 69:C1:402:HEM:HAD2 | 2.51                     | 0.41              |
| 3:C1:257:THR:OG1   | 3:C1:257:THR:O     | 2.38                     | 0.41              |
| 3:C1:300:ILE:HD11  | 3:C1:362:ILE:CG2   | 2.50                     | 0.41              |
| 4:D1:5:LEU:HG      | 4:D1:152:TYR:HE1   | 1.86                     | 0.41              |
| 6:F1:91:GLU:O      | 6:F1:92:PRO:C      | 2.62                     | 0.41              |
| 7:G1:68:LYS:O      | 7:G1:69:SER:C      | 2.64                     | 0.41              |
| 5:Q1:76:ILE:O      | 5:Q1:77:LYS:CG     | 2.68                     | 0.41              |
| 6:R1:52:GLU:HG3    | 6:R1:56:ASN:ND2    | 2.36                     | 0.41              |
| 6:R1:62:ILE:O      | 6:R1:66:LEU:HG     | 2.21                     | 0.41              |
| 9:U1:62:ARG:HB3    | 9:U1:63:PRO:CD     | 2.51                     | 0.41              |
| 14:42:423:ILE:HD12 | 44:a2:56:ARG:HB3   | 2.03                     | 0.41              |
| 73:42:501:CDL:H742 | 73:42:501:CDL:H712 | 1.80                     | 0.41              |
| 34:Q2:53:PRO:HD2   | 39:V2:116:TRP:CD1  | 2.56                     | 0.41              |
| 35:R2:201:ILE:HD12 | 35:R2:201:ILE:HA   | 1.95                     | 0.41              |
| 48:f2:148:GLY:HA3  | 48:f2:149:PRO:HD3  | 1.87                     | 0.41              |
| 52:12:126:LYS:CD   | 52:12:127:TYR:CA   | 2.91                     | 0.41              |
| 52:12:215:TYR:HD1  | 52:12:219:PRO:HB2  | 1.86                     | 0.41              |
| 53:62:3:MET:HA     | 53:62:6:SER:HB2    | 2.02                     | 0.41              |
| 56:A3:276:ALA:O    | 56:A3:280:ILE:HG13 | 2.21                     | 0.41              |
| 59:D3:79:LYS:HZ3   | 66:K3:15:ASN:HD21  | 1.68                     | 0.41              |
| 1:A1:46:ARG:NE     | 1:A1:163:LEU:HD22  | 2.36                     | 0.41              |
| 1:A1:64:PHE:HA     | 1:A1:75:LEU:HD22   | 2.02                     | 0.41              |
| 1:A1:136:GLN:HE21  | 9:I1:50:LEU:CB     | 2.34                     | 0.41              |
| 1:A1:252:HIS:O     | 1:A1:424:GLY:HA2   | 2.20                     | 0.41              |
| 1:A1:282:CYS:SG    | 1:A1:305:GLN:CD    | 3.04                     | 0.41              |
| 1:A1:297:ILE:HG22  | 1:A1:303:LEU:CD1   | 2.49                     | 0.41              |
| 2:B1:68:LEU:HD12   | 2:B1:68:LEU:O      | 2.21                     | 0.41              |
| 2:B1:71:LEU:HA     | 2:B1:71:LEU:HD23   | 1.72                     | 0.41              |
| 2:B1:159:VAL:CG1   | 2:B1:160:ILE:N     | 2.84                     | 0.41              |
| 2:B1:312:PHE:HB3   | 2:B1:323:GLY:O     | 2.20                     | 0.41              |
| 3:C1:1:MET:HG3     | 3:C1:4:ILE:HB      | 2.03                     | 0.41              |
| 3:C1:8:HIS:CB      | 3:C1:9:PRO:HD2     | 2.51                     | 0.41              |
| 3:C1:115:ILE:HG21  | 3:C1:196:HIS:CB    | 2.33                     | 0.41              |
| 3:C1:168:PHE:CE2   | 5:Q1:72:SER:HB2    | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:C1:275:LEU:O     | 3:C1:276:PHE:O    | 2.39                     | 0.41              |
| 4:D1:207:LYS:HB3   | 10:J1:35:PHE:HE2  | 1.85                     | 0.41              |
| 5:E1:20:ASP:O      | 5:E1:22:THR:N     | 2.54                     | 0.41              |
| 6:F1:13:LEU:O      | 6:F1:14:GLU:C     | 2.64                     | 0.41              |
| 6:F1:98:ILE:O      | 6:F1:99:ARG:C     | 2.64                     | 0.41              |
| 7:G1:3:GLN:OE1     | 7:G1:3:GLN:HA     | 2.20                     | 0.41              |
| 8:H1:65:ARG:HG2    | 8:H1:66:ASP:OD2   | 2.21                     | 0.41              |
| 10:J1:29:LEU:O     | 10:J1:30:PHE:C    | 2.64                     | 0.41              |
| 1:M1:32:GLN:HG2    | 1:M1:33:PRO:N     | 2.36                     | 0.41              |
| 1:M1:97:TYR:CD1    | 1:M1:97:TYR:N     | 2.88                     | 0.41              |
| 1:M1:136:GLN:HE21  | 9:U1:50:LEU:HG    | 1.84                     | 0.41              |
| 1:M1:166:SER:CB    | 5:Q1:3:THR:HG22   | 2.51                     | 0.41              |
| 1:M1:244:ARG:NH1   | 7:S1:10:VAL:HB    | 2.36                     | 0.41              |
| 1:M1:248:LEU:HA    | 1:M1:249:PRO:HD3  | 1.78                     | 0.41              |
| 1:M1:289:HIS:O     | 2:N1:87:ARG:NE    | 2.54                     | 0.41              |
| 2:N1:223:PHE:O     | 2:N1:224:LEU:HD23 | 2.21                     | 0.41              |
| 2:N1:396:SER:HA    | 2:N1:399:LEU:HD12 | 2.02                     | 0.41              |
| 2:N1:413:ALA:O     | 2:N1:416:LYS:HB2  | 2.21                     | 0.41              |
| 3:O1:47:THR:O      | 3:O1:48:GLY:C     | 2.64                     | 0.41              |
| 3:O1:207:ASN:O     | 3:O1:208:PRO:C    | 2.62                     | 0.41              |
| 3:O1:241:LEU:HD12  | 3:O1:241:LEU:HA   | 1.81                     | 0.41              |
| 3:O1:303:LEU:HD23  | 3:O1:303:LEU:HA   | 1.85                     | 0.41              |
| 4:P1:21:LEU:CD1    | 4:P1:192:TRP:HB2  | 2.50                     | 0.41              |
| 4:P1:34:LYS:O      | 4:P1:38:SER:HB3   | 2.21                     | 0.41              |
| 5:Q1:16:PRO:O      | 5:Q1:17:GLU:C     | 2.63                     | 0.41              |
| 5:Q1:73:LYS:O      | 5:Q1:74:ILE:HD13  | 2.20                     | 0.41              |
| 5:Q1:113:GLU:O     | 5:Q1:114:VAL:C    | 2.63                     | 0.41              |
| 6:R1:51:PRO:O      | 6:R1:52:GLU:C     | 2.62                     | 0.41              |
| 7:S1:36:ASN:OD1    | 7:S1:39:ARG:NE    | 2.53                     | 0.41              |
| 7:S1:61:TRP:O      | 7:S1:62:GLY:C     | 2.64                     | 0.41              |
| 9:U1:60:ALA:HB3    | 9:U1:63:PRO:O     | 2.21                     | 0.41              |
| 13:32:79:SER:O     | 30:L2:46:ASN:ND2  | 2.50                     | 0.41              |
| 16:72:22:SER:OG    | 16:72:23:LYS:N    | 2.54                     | 0.41              |
| 19:A2:171:THR:HG23 | 19:A2:173:MET:HE2 | 2.03                     | 0.41              |
| 19:A2:643:ARG:HA   | 19:A2:646:LEU:HB2 | 2.03                     | 0.41              |
| 20:B2:246:GLU:HA   | 20:B2:249:LYS:HE3 | 2.02                     | 0.41              |
| 23:E2:127:ALA:HB1  | 23:E2:148:ASP:H   | 1.86                     | 0.41              |
| 29:K2:67:ALA:N     | 29:K2:75:LYS:O    | 2.54                     | 0.41              |
| 30:L2:31:ILE:HG22  | 30:L2:35:LEU:HD11 | 2.03                     | 0.41              |
| 32:O2:18:LYS:HA    | 32:O2:19:PRO:HD3  | 1.93                     | 0.41              |
| 44:a2:79:ASN:HD22  | 55:e2:76:PRO:HD3  | 1.80                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:12:236:ILE:HD12 | 52:12:236:ILE:HA   | 1.97                     | 0.41              |
| 53:62:65:ASN:HB2   | 53:62:78:LEU:HD11  | 2.01                     | 0.41              |
| 53:62:364:LYS:HD3  | 53:62:435:PRO:HB3  | 2.01                     | 0.41              |
| 58:C3:233:PHE:HA   | 58:C3:236:GLU:HG3  | 2.03                     | 0.41              |
| 59:D3:102:TYR:HD2  | 68:M3:35:TYR:HE1   | 1.68                     | 0.41              |
| 59:D3:127:LYS:O    | 59:D3:130:PRO:HD3  | 2.20                     | 0.41              |
| 60:E3:104:LEU:HA   | 60:E3:104:LEU:HD23 | 1.87                     | 0.41              |
| 63:H3:20:PHE:N     | 63:H3:21:PRO:HD3   | 2.35                     | 0.41              |
| 1:A1:62:LEU:HB3    | 1:A1:122:LEU:HD22  | 2.02                     | 0.41              |
| 1:A1:133:VAL:O     | 1:A1:134:ILE:C     | 2.63                     | 0.41              |
| 2:B1:51:ILE:CG2    | 2:B1:199:PHE:HA    | 2.34                     | 0.41              |
| 2:B1:134:ARG:HE    | 2:B1:134:ARG:HB3   | 1.54                     | 0.41              |
| 3:C1:244:LEU:HD11  | 4:D1:204:MET:HE3   | 2.03                     | 0.41              |
| 3:C1:263:ASN:OD1   | 3:C1:264:THR:N     | 2.54                     | 0.41              |
| 3:C1:299:LEU:HD22  | 3:C1:299:LEU:HA    | 1.79                     | 0.41              |
| 4:D1:16:GLY:O      | 4:D1:17:LEU:C      | 2.64                     | 0.41              |
| 10:J1:49:GLY:N     | 10:J1:54:HIS:CD2   | 2.89                     | 0.41              |
| 1:M1:71:PRO:O      | 1:M1:72:GLY:C      | 2.64                     | 0.41              |
| 1:M1:333:ASP:O     | 1:M1:337:VAL:HG23  | 2.21                     | 0.41              |
| 2:N1:24:LEU:CD2    | 2:N1:38:LEU:HD11   | 2.51                     | 0.41              |
| 2:N1:241:GLY:HA2   | 2:N1:423:SER:HB3   | 2.03                     | 0.41              |
| 2:N1:345:LYS:HG2   | 2:N1:418:VAL:HG11  | 2.03                     | 0.41              |
| 3:O1:246:ALA:N     | 3:O1:247:PRO:HD3   | 2.36                     | 0.41              |
| 3:O1:363:LEU:HD12  | 3:O1:363:LEU:HA    | 1.85                     | 0.41              |
| 4:P1:6:HIS:HA      | 4:P1:7:PRO:HD3     | 1.87                     | 0.41              |
| 4:P1:167:GLU:O     | 4:P1:167:GLU:HG2   | 2.20                     | 0.41              |
| 5:Q1:115:SER:C     | 5:Q1:117:LEU:H     | 2.28                     | 0.41              |
| 8:T1:37:LEU:HD21   | 8:T1:58:LEU:CA     | 2.49                     | 0.41              |
| 13:32:2:ASN:OD1    | 13:32:2:ASN:N      | 2.52                     | 0.41              |
| 19:A2:557:ARG:NE   | 38:U2:144:TYR:CZ   | 2.85                     | 0.41              |
| 20:B2:326:CYS:SG   | 20:B2:329:ARG:NH1  | 2.94                     | 0.41              |
| 21:C2:97:PRO:O     | 21:C2:101:PHE:N    | 2.50                     | 0.41              |
| 22:D2:146:GLU:O    | 35:R2:89:TYR:OH    | 2.35                     | 0.41              |
| 77:R2:601:NAP:H3B  | 77:R2:601:NAP:PA   | 2.61                     | 0.41              |
| 38:U2:55:PHE:HB3   | 38:U2:58:ARG:HG3   | 2.03                     | 0.41              |
| 52:12:75:PRO:HG3   | 52:12:223:PHE:CE1  | 2.45                     | 0.41              |
| 55:e2:37:LEU:O     | 55:e2:76:PRO:CB    | 2.69                     | 0.41              |
| 56:A3:168:ILE:CG2  | 56:A3:189:MET:HG3  | 2.51                     | 0.41              |
| 63:H3:65:PRO:HG2   | 63:H3:68:TRP:CG    | 2.55                     | 0.41              |
| 1:A1:43:ALA:HB1    | 1:A1:189:HIS:CB    | 2.51                     | 0.40              |
| 1:A1:256:ALA:HB3   | 1:A1:421:ALA:HB3   | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:266:ASP:OD1   | 1:A1:266:ASP:N     | 2.54                     | 0.40              |
| 1:A1:367:SER:O     | 1:A1:368:HIS:C     | 2.63                     | 0.40              |
| 1:A1:392:LEU:HA    | 1:A1:395:TRP:HD1   | 1.76                     | 0.40              |
| 2:B1:122:PHE:HD1   | 2:B1:122:PHE:HA    | 1.69                     | 0.40              |
| 2:B1:133:ARG:O     | 2:B1:134:ARG:C     | 2.64                     | 0.40              |
| 3:C1:40:CYS:CB     | 3:C1:90:PHE:HD2    | 2.34                     | 0.40              |
| 3:C1:213:SER:C     | 3:C1:215:VAL:N     | 2.79                     | 0.40              |
| 3:C1:226:ILE:HD13  | 3:C1:226:ILE:N     | 2.35                     | 0.40              |
| 3:C1:301:LEU:HA    | 3:C1:304:ILE:CD1   | 2.51                     | 0.40              |
| 4:D1:56:TYR:HD1    | 4:D1:60:GLU:CD     | 2.29                     | 0.40              |
| 7:G1:18:LEU:HD23   | 7:G1:18:LEU:HA     | 1.94                     | 0.40              |
| 1:M1:131:ARG:NH2   | 1:M1:177:LEU:O     | 2.54                     | 0.40              |
| 1:M1:297:ILE:HG22  | 1:M1:303:LEU:CD1   | 2.43                     | 0.40              |
| 2:N1:22:GLN:OE1    | 2:N1:22:GLN:HA     | 2.21                     | 0.40              |
| 2:N1:54:GLY:HA3    | 2:N1:102:ARG:O     | 2.20                     | 0.40              |
| 2:N1:286:LYS:HD3   | 2:N1:287:ARG:HH12  | 1.80                     | 0.40              |
| 3:O1:51:LEU:HD12   | 69:O1:401:HEM:O1D  | 2.21                     | 0.40              |
| 3:O1:63:PHE:CD1    | 3:O1:63:PHE:C      | 2.98                     | 0.40              |
| 3:O1:300:ILE:CD1   | 3:O1:362:ILE:HG21  | 2.50                     | 0.40              |
| 4:P1:224:ARG:HH21  | 7:S1:27:PRO:CD     | 2.34                     | 0.40              |
| 5:Q1:15:ARG:HH21   | 5:Q1:32:ARG:HB2    | 1.85                     | 0.40              |
| 5:Q1:76:ILE:O      | 5:Q1:77:LYS:HE2    | 2.21                     | 0.40              |
| 8:T1:27:LEU:O      | 8:T1:30:CYS:N      | 2.48                     | 0.40              |
| 10:V1:23:THR:HG22  | 10:V1:24:ILE:N     | 2.36                     | 0.40              |
| 12:22:76:ILE:HG21  | 12:22:91:ASN:HD22  | 1.86                     | 0.40              |
| 19:A2:372:PHE:HB3  | 19:A2:532:PRO:HB2  | 2.02                     | 0.40              |
| 20:B2:421:ARG:HH21 | 20:B2:423:LYS:HB2  | 1.86                     | 0.40              |
| 21:C2:90:ILE:HD12  | 21:C2:145:VAL:HG13 | 2.03                     | 0.40              |
| 26:H2:82:GLN:HE21  | 39:V2:98:MET:HB2   | 1.87                     | 0.40              |
| 38:U2:115:PHE:HB3  | 38:U2:117:LEU:HG   | 2.02                     | 0.40              |
| 42:Y2:91:ASP:O     | 42:Y2:93:SER:N     | 2.54                     | 0.40              |
| 43:Z2:64:VAL:HA    | 43:Z2:67:LEU:HG    | 2.02                     | 0.40              |
| 56:A3:440:TYR:CG   | 57:B3:205:SER:HB3  | 2.57                     | 0.40              |
| 62:G3:44:ARG:HA    | 62:G3:45:PRO:HD2   | 1.76                     | 0.40              |
| 1:A1:53:ASN:O      | 1:A1:53:ASN:ND2    | 2.53                     | 0.40              |
| 1:A1:176:LYS:O     | 1:A1:177:LEU:C     | 2.64                     | 0.40              |
| 1:A1:358:LYS:HD2   | 1:A1:402:VAL:HG12  | 2.03                     | 0.40              |
| 1:A1:363:ASN:OD1   | 2:B1:112:LEU:HD23  | 2.21                     | 0.40              |
| 2:B1:53:ALA:HB2    | 2:B1:198:HIS:HB3   | 2.03                     | 0.40              |
| 2:B1:163:LEU:HA    | 2:B1:163:LEU:HD12  | 1.78                     | 0.40              |
| 3:C1:34:GLY:O      | 3:C1:37:LEU:N      | 2.52                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:C1:133:LEU:HA    | 3:C1:175:LEU:HD11 | 2.04                     | 0.40              |
| 3:C1:145:VAL:O     | 3:C1:145:VAL:HG12 | 2.20                     | 0.40              |
| 3:C1:317:PHE:O     | 6:F1:24:ALA:CB    | 2.70                     | 0.40              |
| 4:D1:241:LYS:OXT   | 4:D1:241:LYS:CG   | 2.62                     | 0.40              |
| 7:G1:40:ARG:O      | 7:G1:43:ALA:N     | 2.52                     | 0.40              |
| 9:I1:70:LEU:CG     | 9:I1:72:VAL:H     | 2.34                     | 0.40              |
| 1:M1:4:TYR:HE2     | 1:M1:396:GLU:HG3  | 1.85                     | 0.40              |
| 1:M1:17:SER:HB2    | 1:M1:25:VAL:HB    | 2.03                     | 0.40              |
| 1:M1:42:ASP:O      | 1:M1:42:ASP:CG    | 2.63                     | 0.40              |
| 1:M1:146:ARG:CZ    | 1:M1:308:GLN:HE22 | 2.34                     | 0.40              |
| 1:M1:311:ASN:CG    | 1:M1:320:LEU:CD2  | 2.95                     | 0.40              |
| 1:M1:372:THR:O     | 1:M1:373:THR:C    | 2.62                     | 0.40              |
| 2:N1:38:LEU:O      | 2:N1:40:ASN:N     | 2.54                     | 0.40              |
| 2:N1:57:TYR:O      | 2:N1:233:SER:HB2  | 2.21                     | 0.40              |
| 2:N1:59:ASN:CG     | 2:N1:60:SER:N     | 2.77                     | 0.40              |
| 2:N1:102:ARG:NH1   | 2:N1:175:SER:HA   | 2.37                     | 0.40              |
| 2:N1:158:HIS:ND1   | 2:N1:246:GLU:OE1  | 2.54                     | 0.40              |
| 2:N1:237:ALA:O     | 2:N1:238:LYS:HB2  | 2.20                     | 0.40              |
| 3:O1:115:ILE:O     | 3:O1:116:GLY:C    | 2.64                     | 0.40              |
| 4:P1:7:PRO:HB3     | 4:P1:125:ASP:C    | 2.46                     | 0.40              |
| 4:P1:153:PHE:HA    | 4:P1:154:PRO:HD2  | 1.88                     | 0.40              |
| 4:P1:206:LEU:O     | 4:P1:210:LEU:HD12 | 2.22                     | 0.40              |
| 5:Q1:109:GLU:OE2   | 5:Q1:166:ASP:HB2  | 2.21                     | 0.40              |
| 6:R1:43:VAL:O      | 6:R1:47:ILE:HG13  | 2.22                     | 0.40              |
| 7:S1:50:PRO:O      | 7:S1:53:VAL:HB    | 2.21                     | 0.40              |
| 14:42:285:LEU:O    | 14:42:406:TYR:OH  | 2.32                     | 0.40              |
| 14:42:356:ALA:HA   | 14:42:359:TRP:HD1 | 1.87                     | 0.40              |
| 19:A2:312:GLY:H    | 38:U2:144:TYR:N   | 2.19                     | 0.40              |
| 20:B2:261:MET:HA   | 23:E2:70:LEU:HD21 | 2.03                     | 0.40              |
| 21:C2:220:ARG:NH2  | 32:O2:104:MET:O   | 2.55                     | 0.40              |
| 37:T2:124:LEU:O    | 37:T2:128:GLY:N   | 2.55                     | 0.40              |
| 39:V2:46:GLY:O     | 39:V2:49:SER:OG   | 2.30                     | 0.40              |
| 41:X2:13:HIS:O     | 41:X2:15:LEU:N    | 2.54                     | 0.40              |
| 53:62:387:THR:HG22 | 53:62:462:LEU:HA  | 2.03                     | 0.40              |
| 55:e2:48:ARG:HA    | 55:e2:49:ALA:HA   | 1.59                     | 0.40              |
| 56:A3:34:SER:HB3   | 56:A3:61:HIS:CE1  | 2.57                     | 0.40              |
| 56:A3:442:ASP:OD2  | 57:B3:134:ARG:NH2 | 2.54                     | 0.40              |
| 57:B3:164:ALA:HB2  | 57:B3:171:LYS:HD3 | 2.03                     | 0.40              |
| 58:C3:228:THR:O    | 58:C3:232:HIS:HD2 | 2.04                     | 0.40              |
| 64:I3:29:LEU:HD23  | 64:I3:29:LEU:HA   | 1.85                     | 0.40              |
| 68:M3:37:LEU:HD23  | 68:M3:37:LEU:HA   | 1.83                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B1:303:VAL:HG12  | 2:B1:304:HIS:H     | 1.86                     | 0.40              |
| 2:B1:353:SER:C     | 2:B1:355:PRO:HD2   | 2.47                     | 0.40              |
| 3:C1:48:GLY:HA3    | 69:C1:401:HEM:C3C  | 2.56                     | 0.40              |
| 4:D1:27:ARG:CZ     | 10:J1:58:LYS:HE3   | 2.52                     | 0.40              |
| 4:D1:82:MET:SD     | 4:D1:86:LYS:CD     | 3.08                     | 0.40              |
| 4:D1:99:GLU:H      | 4:D1:99:GLU:HG2    | 1.73                     | 0.40              |
| 4:D1:125:ASP:O     | 4:D1:126:TYR:C     | 2.64                     | 0.40              |
| 4:D1:220:TYR:HD2   | 7:G1:26:PHE:CZ     | 2.40                     | 0.40              |
| 6:F1:93:TYR:O      | 6:F1:97:VAL:HG23   | 2.22                     | 0.40              |
| 10:J1:34:ALA:O     | 10:J1:35:PHE:O     | 2.39                     | 0.40              |
| 10:J1:44:GLU:O     | 10:J1:45:HIS:C     | 2.63                     | 0.40              |
| 2:N1:282:GLY:HA2   | 2:N1:283:PRO:HD2   | 1.78                     | 0.40              |
| 3:O1:75:TYR:CG     | 5:Q1:57:GLN:HG2    | 2.56                     | 0.40              |
| 3:O1:121:LEU:HA    | 3:O1:124:MET:SD    | 2.62                     | 0.40              |
| 4:P1:216:LEU:N     | 4:P1:217:PRO:CD    | 2.85                     | 0.40              |
| 5:Q1:122:HIS:HE1   | 5:Q1:124:LEU:HD12  | 1.85                     | 0.40              |
| 12:22:250:SER:HB2  | 12:22:257:LEU:HD13 | 2.03                     | 0.40              |
| 14:42:274:SER:HA   | 14:42:277:LEU:HD13 | 2.03                     | 0.40              |
| 17:82:198:VAL:HG11 | 17:82:216:ILE:HD11 | 2.03                     | 0.40              |
| 18:92:205:ILE:HG22 | 18:92:209:LYS:HE2  | 2.03                     | 0.40              |
| 20:B2:164:PRO:HA   | 20:B2:165:PRO:HD3  | 1.93                     | 0.40              |
| 37:T2:26:THR:O     | 37:T2:30:GLY:N     | 2.52                     | 0.40              |
| 53:62:192:ASN:HB2  | 53:62:193:LEU:HD12 | 2.03                     | 0.40              |
| 54:g2:145:ASP:O    | 54:g2:148:ALA:N    | 2.54                     | 0.40              |
| 55:e2:124:VAL:HG22 | 55:e2:125:ASN:H    | 1.87                     | 0.40              |
| 56:A3:398:PRO:HB3  | 56:A3:482:VAL:HG21 | 2.03                     | 0.40              |
| 56:A3:498:CYS:HA   | 56:A3:499:PRO:HA   | 1.78                     | 0.40              |
| 59:D3:137:LYS:O    | 59:D3:145:TRP:HE3  | 2.03                     | 0.40              |
| 61:F3:49:VAL:O     | 61:F3:91:LEU:HD12  | 2.21                     | 0.40              |
| 61:F3:77:GLY:O     | 61:F3:90:LYS:NZ    | 2.54                     | 0.40              |
| 62:G3:42:ARG:NH1   | 62:G3:74:ARG:NH2   | 2.68                     | 0.40              |
| 1:A1:8:LEU:HD11    | 1:A1:396:GLU:HG3   | 2.02                     | 0.40              |
| 1:A1:24:ARG:HH11   | 1:A1:24:ARG:HD2    | 1.57                     | 0.40              |
| 2:B1:141:GLN:CB    | 2:B1:142:PRO:HD3   | 2.41                     | 0.40              |
| 2:B1:156:GLN:O     | 2:B1:157:ALA:C     | 2.63                     | 0.40              |
| 2:B1:194:TYR:O     | 2:B1:195:VAL:C     | 2.64                     | 0.40              |
| 2:B1:346:THR:HG23  | 2:B1:351:ASN:HB3   | 2.03                     | 0.40              |
| 2:B1:408:ALA:O     | 2:B1:411:ILE:N     | 2.54                     | 0.40              |
| 3:C1:170:VAL:O     | 3:C1:170:VAL:CG1   | 2.68                     | 0.40              |
| 3:C1:274:PHE:O     | 3:C1:275:LEU:C     | 2.62                     | 0.40              |
| 3:C1:341:GLN:OE1   | 3:C1:347:TYR:CZ    | 2.74                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D1:35:GLN:HB2    | 4:D1:169:LEU:HD13  | 2.02                     | 0.40              |
| 4:D1:95:TYR:CD1    | 4:D1:95:TYR:N      | 2.90                     | 0.40              |
| 4:D1:146:GLY:O     | 4:D1:148:TYR:HD1   | 2.04                     | 0.40              |
| 4:D1:165:TYR:HD1   | 4:D1:166:ASN:O     | 2.04                     | 0.40              |
| 8:H1:50:THR:CG2    | 8:H1:51:GLU:N      | 2.83                     | 0.40              |
| 1:M1:85:HIS:CE1    | 2:N1:284:HIS:ND1   | 2.90                     | 0.40              |
| 1:M1:349:ALA:O     | 1:M1:408:ARG:NE    | 2.54                     | 0.40              |
| 2:N1:92:VAL:HG11   | 2:N1:115:ASP:CB    | 2.51                     | 0.40              |
| 2:N1:257:LEU:HD13  | 2:N1:424:MET:CB    | 2.45                     | 0.40              |
| 2:N1:276:GLN:OE1   | 9:U1:59:ALA:HB1    | 2.21                     | 0.40              |
| 3:O1:25:SER:HA     | 3:O1:218:ILE:HD12  | 2.02                     | 0.40              |
| 3:O1:156:ILE:H     | 3:O1:156:ILE:HG12  | 1.63                     | 0.40              |
| 4:P1:43:MET:HG2    | 4:P1:114:SER:N     | 2.37                     | 0.40              |
| 6:R1:99:ARG:O      | 6:R1:100:GLU:C     | 2.63                     | 0.40              |
| 10:V1:2:ALA:HB1    | 10:V1:3:PRO:HD2    | 2.03                     | 0.40              |
| 14:42:457:PRO:HG2  | 14:42:458:LEU:HA   | 2.04                     | 0.40              |
| 19:A2:170:LYS:HB3  | 19:A2:232:THR:HG23 | 2.02                     | 0.40              |
| 19:A2:312:GLY:CA   | 38:U2:144:TYR:N    | 2.82                     | 0.40              |
| 19:A2:445:LEU:HD21 | 19:A2:460:HIS:HD2  | 1.87                     | 0.40              |
| 29:K2:31:GLN:HB3   | 29:K2:34:ARG:HH21  | 1.86                     | 0.40              |
| 35:R2:322:ILE:H    | 35:R2:322:ILE:HG13 | 1.72                     | 0.40              |
| 45:b2:166:GLY:HA2  | 45:b2:167:PRO:HD3  | 1.86                     | 0.40              |
| 53:62:141:PHE:HB2  | 53:62:182:PHE:HE2  | 1.86                     | 0.40              |
| 57:B3:86:MET:HE3   | 57:B3:86:MET:HB2   | 1.80                     | 0.40              |
| 66:K3:24:PHE:CE1   | 66:K3:28:VAL:HG21  | 2.56                     | 0.40              |
| 1:A1:50:GLU:O      | 1:A1:173:ASN:ND2   | 2.55                     | 0.40              |
| 1:A1:213:GLN:CB    | 1:A1:215:HIS:CD2   | 3.05                     | 0.40              |
| 2:B1:213:HIS:O     | 2:B1:213:HIS:CD2   | 2.74                     | 0.40              |
| 3:C1:68:HIS:NE2    | 5:E1:67:ASP:CB     | 2.85                     | 0.40              |
| 3:C1:192:ILE:O     | 3:C1:193:ALA:C     | 2.62                     | 0.40              |
| 4:D1:136:GLU:O     | 4:D1:137:PRO:C     | 2.62                     | 0.40              |
| 4:D1:200:HIS:O     | 4:D1:203:ARG:HB3   | 2.20                     | 0.40              |
| 5:E1:53:ASN:O      | 5:E1:54:VAL:C      | 2.65                     | 0.40              |
| 11:K1:27:VAL:HG12  | 11:K1:28:GLY:N     | 2.37                     | 0.40              |
| 1:M1:241:ILE:HD11  | 7:S1:16:TYR:CE2    | 2.55                     | 0.40              |
| 2:N1:207:ILE:HD12  | 2:N1:382:VAL:HG12  | 2.04                     | 0.40              |
| 3:O1:66:VAL:O      | 3:O1:69:ILE:HB     | 2.21                     | 0.40              |
| 3:O1:227:LYS:HG3   | 4:P1:223:LYS:NZ    | 2.36                     | 0.40              |
| 3:O1:297:SER:O     | 3:O1:300:ILE:CG2   | 2.62                     | 0.40              |
| 4:P1:14:HIS:HA     | 4:P1:19:SER:CB     | 2.51                     | 0.40              |
| 4:P1:175:THR:HA    | 4:P1:176:PRO:HD2   | 1.71                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:P1:301:HEC:HHD  | 70:P1:301:HEC:CBC  | 2.30                     | 0.40              |
| 5:Q1:83:GLU:HA     | 5:Q1:100:HIS:CG    | 2.57                     | 0.40              |
| 6:R1:91:GLU:O      | 6:R1:95:LYS:HG3    | 2.21                     | 0.40              |
| 9:U1:70:LEU:HD11   | 9:U1:72:VAL:H      | 1.85                     | 0.40              |
| 10:V1:42:ILE:O     | 10:V1:46:ILE:HG12  | 2.22                     | 0.40              |
| 12:22:45:MET:HE1   | 12:22:53:THR:HA    | 2.02                     | 0.40              |
| 14:42:35:SER:O     | 14:42:38:SER:OG    | 2.35                     | 0.40              |
| 14:42:348:LEU:HG   | 14:42:349:GLN:H    | 1.87                     | 0.40              |
| 15:52:26:LEU:HB3   | 15:52:88:ASP:HB2   | 2.04                     | 0.40              |
| 17:82:270:ASN:HD21 | 17:82:338:ASP:HA   | 1.86                     | 0.40              |
| 19:A2:413:LEU:HD23 | 19:A2:413:LEU:HA   | 1.92                     | 0.40              |
| 21:C2:205:PRO:HA   | 25:G2:124:LEU:HD21 | 2.03                     | 0.40              |
| 26:H2:15:ASP:OD1   | 26:H2:15:ASP:N     | 2.52                     | 0.40              |
| 27:I2:87:CYS:HB3   | 76:I2:300:ZN:ZN    | 1.52                     | 0.40              |
| 30:L2:80:TRP:O     | 30:L2:84:LEU:N     | 2.54                     | 0.40              |
| 53:62:107:TYR:HE2  | 53:62:240:PRO:HB3  | 1.87                     | 0.40              |
| 56:A3:240:HIS:O    | 56:A3:241:PRO:C    | 2.64                     | 0.40              |
| 56:A3:373:VAL:O    | 56:A3:377:PHE:CD2  | 2.75                     | 0.40              |
| 56:A3:430:PHE:O    | 56:A3:431:LEU:C    | 2.64                     | 0.40              |
| 57:B3:215:PRO:HD3  | 64:I3:60:PHE:CD1   | 2.57                     | 0.40              |
| 63:H3:17:ASP:OD1   | 63:H3:19:ARG:HG2   | 2.22                     | 0.40              |
| 65:J3:5:VAL:O      | 65:J3:9:GLN:HG3    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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   | A1    | 428/480 (89%) | 348 (81%) | 57 (13%) | 23 (5%)  | 1           | 15 |
| 1   | M1    | 428/480 (89%) | 360 (84%) | 50 (12%) | 18 (4%)  | 2           | 17 |
| 2   | B1    | 417/453 (92%) | 341 (82%) | 67 (16%) | 9 (2%)   | 5           | 29 |

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| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|-----------|----------|-------------|-----|
| 2   | N1    | 417/453 (92%)  | 344 (82%) | 62 (15%)  | 11 (3%)  | 4           | 25  |
| 3   | C1    | 377/379 (100%) | 303 (80%) | 60 (16%)  | 14 (4%)  | 2           | 20  |
| 3   | O1    | 377/379 (100%) | 316 (84%) | 50 (13%)  | 11 (3%)  | 3           | 23  |
| 4   | D1    | 239/325 (74%)  | 188 (79%) | 36 (15%)  | 15 (6%)  | 1           | 13  |
| 4   | P1    | 239/325 (74%)  | 195 (82%) | 32 (13%)  | 12 (5%)  | 1           | 16  |
| 5   | E1    | 73/196 (37%)   | 57 (78%)  | 14 (19%)  | 2 (3%)   | 4           | 25  |
| 5   | Q1    | 194/196 (99%)  | 149 (77%) | 34 (18%)  | 11 (6%)  | 1           | 14  |
| 6   | F1    | 104/111 (94%)  | 89 (86%)  | 12 (12%)  | 3 (3%)   | 3           | 23  |
| 6   | R1    | 104/111 (94%)  | 86 (83%)  | 16 (15%)  | 2 (2%)   | 6           | 32  |
| 7   | G1    | 79/82 (96%)    | 63 (80%)  | 13 (16%)  | 3 (4%)   | 2           | 19  |
| 7   | S1    | 79/82 (96%)    | 60 (76%)  | 16 (20%)  | 3 (4%)   | 2           | 19  |
| 8   | H1    | 62/91 (68%)    | 52 (84%)  | 10 (16%)  | 0        | 100         | 100 |
| 8   | T1    | 62/91 (68%)    | 51 (82%)  | 10 (16%)  | 1 (2%)   | 7           | 38  |
| 9   | I1    | 31/78 (40%)    | 19 (61%)  | 10 (32%)  | 2 (6%)   | 1           | 12  |
| 9   | U1    | 31/78 (40%)    | 17 (55%)  | 11 (36%)  | 3 (10%)  | 0           | 7   |
| 10  | J1    | 60/64 (94%)    | 41 (68%)  | 13 (22%)  | 6 (10%)  | 0           | 7   |
| 10  | V1    | 60/64 (94%)    | 45 (75%)  | 11 (18%)  | 4 (7%)   | 1           | 12  |
| 11  | K1    | 20/56 (36%)    | 17 (85%)  | 2 (10%)   | 1 (5%)   | 1           | 16  |
| 11  | W1    | 20/56 (36%)    | 17 (85%)  | 3 (15%)   | 0        | 100         | 100 |
| 12  | 22    | 342/347 (99%)  | 295 (86%) | 47 (14%)  | 0        | 100         | 100 |
| 13  | 32    | 89/115 (77%)   | 74 (83%)  | 14 (16%)  | 1 (1%)   | 11          | 46  |
| 14  | 42    | 457/459 (100%) | 383 (84%) | 70 (15%)  | 4 (1%)   | 14          | 51  |
| 15  | 52    | 94/98 (96%)    | 82 (87%)  | 12 (13%)  | 0        | 100         | 100 |
| 16  | 72    | 170/175 (97%)  | 140 (82%) | 28 (16%)  | 2 (1%)   | 10          | 44  |
| 17  | 82    | 425/444 (96%)  | 346 (81%) | 78 (18%)  | 1 (0%)   | 43          | 78  |
| 18  | 92    | 205/217 (94%)  | 169 (82%) | 35 (17%)  | 1 (0%)   | 24          | 63  |
| 19  | A2    | 686/704 (97%)  | 572 (83%) | 107 (16%) | 7 (1%)   | 12          | 49  |
| 20  | B2    | 383/430 (89%)  | 334 (87%) | 40 (10%)  | 9 (2%)   | 5           | 28  |
| 21  | C2    | 206/228 (90%)  | 177 (86%) | 29 (14%)  | 0        | 100         | 100 |
| 22  | D2    | 150/179 (84%)  | 130 (87%) | 19 (13%)  | 1 (1%)   | 18          | 56  |
| 23  | E2    | 174/176 (99%)  | 158 (91%) | 15 (9%)   | 1 (1%)   | 21          | 59  |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 24  | F2    | 26/75 (35%)    | 19 (73%)  | 7 (27%)  | 0        | 100         | 100 |
| 25  | G2    | 121/133 (91%)  | 100 (83%) | 20 (16%) | 1 (1%)   | 16          | 54  |
| 26  | H2    | 94/105 (90%)   | 73 (78%)  | 21 (22%) | 0        | 100         | 100 |
| 27  | I2    | 69/96 (72%)    | 53 (77%)  | 14 (20%) | 2 (3%)   | 3           | 23  |
| 28  | J2    | 67/70 (96%)    | 61 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 29  | K2    | 82/98 (84%)    | 63 (77%)  | 19 (23%) | 0        | 100         | 100 |
| 30  | L2    | 78/83 (94%)    | 66 (85%)  | 12 (15%) | 0        | 100         | 100 |
| 31  | N2    | 109/115 (95%)  | 93 (85%)  | 16 (15%) | 0        | 100         | 100 |
| 32  | O2    | 112/127 (88%)  | 97 (87%)  | 15 (13%) | 0        | 100         | 100 |
| 33  | P2    | 86/112 (77%)   | 64 (74%)  | 22 (26%) | 0        | 100         | 100 |
| 34  | Q2    | 166/171 (97%)  | 126 (76%) | 40 (24%) | 0        | 100         | 100 |
| 35  | R2    | 302/345 (88%)  | 241 (80%) | 59 (20%) | 2 (1%)   | 18          | 56  |
| 36  | S2    | 317/320 (99%)  | 246 (78%) | 69 (22%) | 2 (1%)   | 21          | 59  |
| 37  | T2    | 136/140 (97%)  | 116 (85%) | 20 (15%) | 0        | 100         | 100 |
| 38  | U2    | 87/145 (60%)   | 63 (72%)  | 24 (28%) | 0        | 100         | 100 |
| 39  | V2    | 136/143 (95%)  | 121 (89%) | 14 (10%) | 1 (1%)   | 18          | 56  |
| 40  | M2    | 78/88 (89%)    | 62 (80%)  | 16 (20%) | 0        | 100         | 100 |
| 40  | W2    | 79/88 (90%)    | 68 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 41  | X2    | 47/57 (82%)    | 38 (81%)  | 8 (17%)  | 1 (2%)   | 5           | 30  |
| 42  | Y2    | 55/72 (76%)    | 46 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 43  | Z2    | 72/97 (74%)    | 57 (79%)  | 15 (21%) | 0        | 100         | 100 |
| 44  | a2    | 112/128 (88%)  | 95 (85%)  | 17 (15%) | 0        | 100         | 100 |
| 45  | b2    | 137/143 (96%)  | 113 (82%) | 24 (18%) | 0        | 100         | 100 |
| 46  | c2    | 86/127 (68%)   | 68 (79%)  | 18 (21%) | 0        | 100         | 100 |
| 47  | d2    | 105/136 (77%)  | 82 (78%)  | 21 (20%) | 2 (2%)   | 6           | 32  |
| 48  | f2    | 165/178 (93%)  | 135 (82%) | 30 (18%) | 0        | 100         | 100 |
| 49  | h2    | 89/125 (71%)   | 62 (70%)  | 25 (28%) | 2 (2%)   | 5           | 29  |
| 50  | i2    | 36/49 (74%)    | 35 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 51  | j2    | 111/120 (92%)  | 92 (83%)  | 19 (17%) | 0        | 100         | 100 |
| 52  | 12    | 305/318 (96%)  | 269 (88%) | 34 (11%) | 2 (1%)   | 18          | 56  |
| 53  | 62    | 604/606 (100%) | 536 (89%) | 67 (11%) | 1 (0%)   | 43          | 78  |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 54  | g2    | 171/176 (97%)     | 139 (81%)   | 32 (19%)   | 0        | 100         | 100 |
| 55  | e2    | 139/158 (88%)     | 82 (59%)    | 50 (36%)   | 7 (5%)   | 1           | 16  |
| 56  | A3    | 512/514 (100%)    | 479 (94%)   | 29 (6%)    | 4 (1%)   | 16          | 54  |
| 57  | B3    | 225/227 (99%)     | 203 (90%)   | 19 (8%)    | 3 (1%)   | 9           | 42  |
| 58  | C3    | 259/261 (99%)     | 249 (96%)   | 10 (4%)    | 0        | 100         | 100 |
| 59  | D3    | 142/169 (84%)     | 135 (95%)   | 7 (5%)     | 0        | 100         | 100 |
| 60  | E3    | 107/152 (70%)     | 104 (97%)   | 3 (3%)     | 0        | 100         | 100 |
| 61  | F3    | 96/129 (74%)      | 86 (90%)    | 6 (6%)     | 4 (4%)   | 2           | 17  |
| 62  | G3    | 82/97 (84%)       | 67 (82%)    | 10 (12%)   | 5 (6%)   | 1           | 13  |
| 63  | H3    | 73/86 (85%)       | 64 (88%)    | 8 (11%)    | 1 (1%)   | 9           | 40  |
| 64  | I3    | 71/74 (96%)       | 65 (92%)    | 6 (8%)     | 0        | 100         | 100 |
| 65  | J3    | 54/80 (68%)       | 48 (89%)    | 4 (7%)     | 2 (4%)   | 2           | 20  |
| 66  | K3    | 47/80 (59%)       | 41 (87%)    | 6 (13%)    | 0        | 100         | 100 |
| 67  | L3    | 45/63 (71%)       | 42 (93%)    | 3 (7%)     | 0        | 100         | 100 |
| 68  | M3    | 41/70 (59%)       | 39 (95%)    | 2 (5%)     | 0        | 100         | 100 |
| All | All   | 13415/15148 (89%) | 11221 (84%) | 1971 (15%) | 223 (2%) | 9           | 36  |

All (223) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 327 | ASP  |
| 1   | A1    | 426 | GLY  |
| 1   | A1    | 427 | PRO  |
| 2   | B1    | 141 | GLN  |
| 2   | B1    | 183 | ILE  |
| 2   | B1    | 305 | GLN  |
| 3   | C1    | 8   | HIS  |
| 3   | C1    | 27  | ILE  |
| 3   | C1    | 109 | PHE  |
| 4   | D1    | 51  | LEU  |
| 4   | D1    | 73  | GLY  |
| 4   | D1    | 98  | PRO  |
| 9   | I1    | 72  | VAL  |
| 1   | M1    | 55  | ALA  |
| 1   | M1    | 427 | PRO  |
| 2   | N1    | 141 | GLN  |
| 2   | N1    | 183 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N1    | 351 | ASN  |
| 3   | O1    | 8   | HIS  |
| 3   | O1    | 27  | ILE  |
| 3   | O1    | 157 | GLY  |
| 4   | P1    | 51  | LEU  |
| 4   | P1    | 73  | GLY  |
| 5   | Q1    | 114 | VAL  |
| 5   | Q1    | 141 | HIS  |
| 9   | U1    | 72  | VAL  |
| 10  | V1    | 58  | LYS  |
| 19  | A2    | 463 | SER  |
| 20  | B2    | 88  | HIS  |
| 20  | B2    | 294 | ARG  |
| 27  | I2    | 105 | LYS  |
| 36  | S2    | 200 | PRO  |
| 36  | S2    | 276 | ASP  |
| 47  | d2    | 40  | VAL  |
| 49  | h2    | 81  | ALA  |
| 49  | h2    | 82  | VAL  |
| 52  | l2    | 126 | LYS  |
| 55  | e2    | 68  | ASP  |
| 55  | e2    | 71  | GLY  |
| 55  | e2    | 81  | ARG  |
| 55  | e2    | 82  | SER  |
| 56  | A3    | 328 | HIS  |
| 56  | A3    | 508 | PRO  |
| 61  | F3    | 2   | SER  |
| 61  | F3    | 87  | THR  |
| 61  | F3    | 95  | GLN  |
| 62  | G3    | 4   | ALA  |
| 62  | G3    | 9   | GLY  |
| 63  | H3    | 46  | LYS  |
| 65  | J3    | 2   | GLU  |
| 1   | A1    | 55  | ALA  |
| 1   | A1    | 56  | GLY  |
| 1   | A1    | 72  | GLY  |
| 1   | A1    | 80  | GLU  |
| 1   | A1    | 81  | SER  |
| 1   | A1    | 287 | GLY  |
| 1   | A1    | 288 | ALA  |
| 1   | A1    | 342 | TRP  |
| 2   | B1    | 236 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B1    | 351 | ASN  |
| 3   | C1    | 28  | SER  |
| 3   | C1    | 137 | GLN  |
| 3   | C1    | 157 | GLY  |
| 3   | C1    | 313 | ARG  |
| 4   | D1    | 154 | PRO  |
| 7   | G1    | 68  | LYS  |
| 9   | I1    | 59  | ALA  |
| 10  | J1    | 58  | LYS  |
| 11  | K1    | 33  | VAL  |
| 1   | M1    | 52  | ASN  |
| 1   | M1    | 72  | GLY  |
| 1   | M1    | 246 | ASP  |
| 1   | M1    | 282 | CYS  |
| 1   | M1    | 385 | THR  |
| 2   | N1    | 236 | LYS  |
| 5   | Q1    | 137 | GLY  |
| 9   | U1    | 59  | ALA  |
| 10  | V1    | 23  | THR  |
| 10  | V1    | 24  | ILE  |
| 16  | 72    | 171 | ILE  |
| 20  | B2    | 84  | PHE  |
| 20  | B2    | 91  | ALA  |
| 20  | B2    | 93  | GLY  |
| 20  | B2    | 94  | VAL  |
| 22  | D2    | 113 | PHE  |
| 27  | I2    | 107 | THR  |
| 41  | X2    | 14  | VAL  |
| 52  | 12    | 282 | TYR  |
| 55  | e2    | 74  | ASP  |
| 55  | e2    | 76  | PRO  |
| 62  | G3    | 5   | LYS  |
| 1   | A1    | 52  | ASN  |
| 1   | A1    | 352 | SER  |
| 1   | A1    | 385 | THR  |
| 1   | A1    | 395 | TRP  |
| 2   | B1    | 91  | ALA  |
| 3   | C1    | 283 | SER  |
| 3   | C1    | 319 | PRO  |
| 4   | D1    | 27  | ARG  |
| 4   | D1    | 119 | ALA  |
| 4   | D1    | 162 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D1    | 218 | LEU  |
| 5   | E1    | 16  | PRO  |
| 5   | E1    | 72  | SER  |
| 10  | J1    | 23  | THR  |
| 10  | J1    | 35  | PHE  |
| 1   | M1    | 81  | SER  |
| 1   | M1    | 107 | PRO  |
| 1   | M1    | 426 | GLY  |
| 2   | N1    | 24  | LEU  |
| 2   | N1    | 305 | GLN  |
| 3   | O1    | 28  | SER  |
| 3   | O1    | 62  | ALA  |
| 3   | O1    | 316 | MET  |
| 3   | O1    | 319 | PRO  |
| 4   | P1    | 80  | MET  |
| 4   | P1    | 162 | PRO  |
| 5   | Q1    | 64  | ALA  |
| 5   | Q1    | 177 | PRO  |
| 7   | S1    | 68  | LYS  |
| 10  | V1    | 57  | HIS  |
| 14  | 42    | 20  | ASN  |
| 14  | 42    | 21  | ASN  |
| 14  | 42    | 419 | TYR  |
| 16  | 72    | 149 | TYR  |
| 19  | A2    | 365 | THR  |
| 19  | A2    | 383 | SER  |
| 20  | B2    | 85  | GLY  |
| 25  | G2    | 122 | SER  |
| 35  | R2    | 134 | TRP  |
| 35  | R2    | 272 | LEU  |
| 57  | B3    | 104 | TRP  |
| 62  | G3    | 61  | SER  |
| 1   | A1    | 107 | PRO  |
| 1   | A1    | 246 | ASP  |
| 1   | A1    | 391 | PRO  |
| 3   | C1    | 236 | ILE  |
| 3   | C1    | 365 | LEU  |
| 4   | D1    | 80  | MET  |
| 6   | F1    | 95  | LYS  |
| 10  | J1    | 4   | THR  |
| 10  | J1    | 57  | HIS  |
| 1   | M1    | 6   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M1    | 109 | ALA  |
| 2   | N1    | 269 | ALA  |
| 2   | N1    | 409 | ASP  |
| 3   | O1    | 24  | PRO  |
| 3   | O1    | 109 | PHE  |
| 5   | Q1    | 130 | PRO  |
| 6   | R1    | 95  | LYS  |
| 17  | 82    | 227 | PRO  |
| 18  | 92    | 76  | ALA  |
| 19  | A2    | 563 | ASP  |
| 39  | V2    | 143 | TYR  |
| 47  | d2    | 19  | PRO  |
| 56  | A3    | 51  | ASP  |
| 1   | A1    | 6   | GLN  |
| 1   | A1    | 152 | TYR  |
| 2   | B1    | 39  | GLU  |
| 3   | C1    | 316 | MET  |
| 4   | D1    | 147 | LEU  |
| 7   | G1    | 72  | LYS  |
| 1   | M1    | 338 | LEU  |
| 1   | M1    | 391 | PRO  |
| 3   | O1    | 247 | PRO  |
| 3   | O1    | 255 | ASN  |
| 4   | P1    | 83  | ARG  |
| 4   | P1    | 98  | PRO  |
| 4   | P1    | 110 | PRO  |
| 4   | P1    | 147 | LEU  |
| 4   | P1    | 154 | PRO  |
| 5   | Q1    | 16  | PRO  |
| 5   | Q1    | 43  | THR  |
| 5   | Q1    | 69  | LEU  |
| 5   | Q1    | 188 | THR  |
| 7   | S1    | 50  | PRO  |
| 14  | 42    | 112 | ALA  |
| 19  | A2    | 541 | PRO  |
| 20  | B2    | 291 | VAL  |
| 23  | E2    | 108 | SER  |
| 57  | B3    | 103 | GLN  |
| 65  | J3    | 3   | ASN  |
| 1   | A1    | 33  | PRO  |
| 1   | A1    | 109 | ALA  |
| 2   | B1    | 52  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D1    | 110 | PRO  |
| 4   | D1    | 163 | PRO  |
| 4   | D1    | 176 | PRO  |
| 7   | G1    | 45  | ILE  |
| 1   | M1    | 185 | TYR  |
| 2   | N1    | 52  | LYS  |
| 4   | P1    | 176 | PRO  |
| 53  | 62    | 31  | ASN  |
| 56  | A3    | 91  | ASP  |
| 57  | B3    | 158 | ASP  |
| 62  | G3    | 49  | PRO  |
| 2   | B1    | 129 | ALA  |
| 6   | F1    | 51  | PRO  |
| 1   | M1    | 56  | GLY  |
| 1   | M1    | 293 | PRO  |
| 20  | B2    | 219 | GLY  |
| 3   | C1    | 339 | GLY  |
| 4   | D1    | 83  | ARG  |
| 2   | N1    | 85  | ILE  |
| 2   | N1    | 109 | VAL  |
| 5   | Q1    | 84  | GLY  |
| 8   | T1    | 69  | VAL  |
| 10  | J1    | 24  | ILE  |
| 4   | P1    | 123 | GLY  |
| 6   | R1    | 51  | PRO  |
| 7   | S1    | 45  | ILE  |
| 13  | 32    | 24  | LEU  |
| 61  | F3    | 15  | GLY  |
| 1   | A1    | 260 | PRO  |
| 4   | D1    | 26  | ILE  |
| 4   | P1    | 163 | PRO  |
| 9   | U1    | 65  | VAL  |
| 19  | A2    | 461 | PRO  |
| 3   | C1    | 372 | ILE  |
| 6   | F1    | 47  | ILE  |
| 19  | A2    | 129 | PRO  |
| 55  | e2    | 78  | LEU  |
| 1   | M1    | 193 | PRO  |

### 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   | A1    | 358/394 (91%)  | 269 (75%)  | 89 (25%) | 0           | 4   |
| 1   | M1    | 358/394 (91%)  | 276 (77%)  | 82 (23%) | 1           | 6   |
| 2   | B1    | 328/355 (92%)  | 254 (77%)  | 74 (23%) | 1           | 6   |
| 2   | N1    | 328/355 (92%)  | 254 (77%)  | 74 (23%) | 1           | 6   |
| 3   | C1    | 327/327 (100%) | 251 (77%)  | 76 (23%) | 1           | 5   |
| 3   | O1    | 327/327 (100%) | 259 (79%)  | 68 (21%) | 1           | 6   |
| 4   | D1    | 206/257 (80%)  | 172 (84%)  | 34 (16%) | 2           | 10  |
| 4   | P1    | 206/257 (80%)  | 170 (82%)  | 36 (18%) | 2           | 9   |
| 5   | E1    | 65/168 (39%)   | 47 (72%)   | 18 (28%) | 0           | 3   |
| 5   | Q1    | 167/168 (99%)  | 110 (66%)  | 57 (34%) | 0           | 1   |
| 6   | F1    | 96/99 (97%)    | 68 (71%)   | 28 (29%) | 0           | 2   |
| 6   | R1    | 96/99 (97%)    | 76 (79%)   | 20 (21%) | 1           | 6   |
| 7   | G1    | 71/72 (99%)    | 53 (75%)   | 18 (25%) | 0           | 3   |
| 7   | S1    | 71/72 (99%)    | 51 (72%)   | 20 (28%) | 0           | 3   |
| 8   | H1    | 61/85 (72%)    | 50 (82%)   | 11 (18%) | 2           | 9   |
| 8   | T1    | 61/85 (72%)    | 50 (82%)   | 11 (18%) | 2           | 9   |
| 9   | I1    | 27/60 (45%)    | 18 (67%)   | 9 (33%)  | 0           | 2   |
| 9   | U1    | 27/60 (45%)    | 19 (70%)   | 8 (30%)  | 0           | 2   |
| 10  | J1    | 52/54 (96%)    | 43 (83%)   | 9 (17%)  | 2           | 9   |
| 10  | V1    | 52/54 (96%)    | 42 (81%)   | 10 (19%) | 1           | 8   |
| 11  | K1    | 15/46 (33%)    | 11 (73%)   | 4 (27%)  | 0           | 3   |
| 11  | W1    | 15/46 (33%)    | 10 (67%)   | 5 (33%)  | 0           | 2   |
| 12  | 22    | 274/316 (87%)  | 274 (100%) | 0        | 100         | 100 |
| 13  | 32    | 75/101 (74%)   | 75 (100%)  | 0        | 100         | 100 |
| 14  | 42    | 351/413 (85%)  | 351 (100%) | 0        | 100         | 100 |
| 15  | 52    | 75/86 (87%)    | 75 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 16  | 72    | 104/142 (73%) | 104 (100%) | 0        | 100         | 100 |
| 17  | 82    | 236/353 (67%) | 236 (100%) | 0        | 100         | 100 |
| 18  | 92    | 160/183 (87%) | 159 (99%)  | 1 (1%)   | 78          | 83  |
| 19  | A2    | 551/588 (94%) | 548 (100%) | 3 (0%)   | 81          | 83  |
| 20  | B2    | 330/371 (89%) | 324 (98%)  | 6 (2%)   | 51          | 68  |
| 21  | C2    | 183/204 (90%) | 182 (100%) | 1 (0%)   | 81          | 83  |
| 22  | D2    | 126/150 (84%) | 123 (98%)  | 3 (2%)   | 43          | 64  |
| 23  | E2    | 145/151 (96%) | 144 (99%)  | 1 (1%)   | 76          | 81  |
| 24  | F2    | 13/69 (19%)   | 13 (100%)  | 0        | 100         | 100 |
| 25  | G2    | 105/119 (88%) | 105 (100%) | 0        | 100         | 100 |
| 26  | H2    | 80/95 (84%)   | 80 (100%)  | 0        | 100         | 100 |
| 27  | I2    | 53/79 (67%)   | 49 (92%)   | 4 (8%)   | 12          | 33  |
| 28  | J2    | 50/59 (85%)   | 50 (100%)  | 0        | 100         | 100 |
| 29  | K2    | 66/81 (82%)   | 66 (100%)  | 0        | 100         | 100 |
| 30  | L2    | 63/71 (89%)   | 63 (100%)  | 0        | 100         | 100 |
| 31  | N2    | 88/101 (87%)  | 88 (100%)  | 0        | 100         | 100 |
| 32  | O2    | 95/113 (84%)  | 95 (100%)  | 0        | 100         | 100 |
| 33  | P2    | 72/96 (75%)   | 72 (100%)  | 0        | 100         | 100 |
| 34  | Q2    | 142/154 (92%) | 140 (99%)  | 2 (1%)   | 59          | 72  |
| 35  | R2    | 230/298 (77%) | 229 (100%) | 1 (0%)   | 84          | 84  |
| 36  | S2    | 205/283 (72%) | 203 (99%)  | 2 (1%)   | 68          | 78  |
| 37  | T2    | 79/101 (78%)  | 79 (100%)  | 0        | 100         | 100 |
| 38  | U2    | 71/131 (54%)  | 71 (100%)  | 0        | 100         | 100 |
| 39  | V2    | 107/120 (89%) | 107 (100%) | 0        | 100         | 100 |
| 40  | M2    | 73/81 (90%)   | 73 (100%)  | 0        | 100         | 100 |
| 40  | W2    | 55/81 (68%)   | 55 (100%)  | 0        | 100         | 100 |
| 41  | X2    | 32/54 (59%)   | 32 (100%)  | 0        | 100         | 100 |
| 42  | Y2    | 29/62 (47%)   | 29 (100%)  | 0        | 100         | 100 |
| 43  | Z2    | 28/75 (37%)   | 28 (100%)  | 0        | 100         | 100 |
| 44  | a2    | 70/114 (61%)  | 69 (99%)   | 1 (1%)   | 59          | 72  |
| 45  | b2    | 85/124 (68%)  | 85 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|-------------|-----|
| 46  | c2    | 45/121 (37%)      | 45 (100%)  | 0        | 100         | 100 |
| 47  | d2    | 42/119 (35%)      | 42 (100%)  | 0        | 100         | 100 |
| 48  | f2    | 80/160 (50%)      | 80 (100%)  | 0        | 100         | 100 |
| 49  | h2    | 70/112 (62%)      | 70 (100%)  | 0        | 100         | 100 |
| 50  | i2    | 23/45 (51%)       | 23 (100%)  | 0        | 100         | 100 |
| 51  | j2    | 88/106 (83%)      | 88 (100%)  | 0        | 100         | 100 |
| 52  | 12    | 267/275 (97%)     | 259 (97%)  | 8 (3%)   | 36          | 57  |
| 53  | 62    | 523/534 (98%)     | 522 (100%) | 1 (0%)   | 87          | 87  |
| 54  | g2    | 130/157 (83%)     | 130 (100%) | 0        | 100         | 100 |
| 55  | e2    | 44/141 (31%)      | 43 (98%)   | 1 (2%)   | 44          | 64  |
| 56  | A3    | 427/427 (100%)    | 387 (91%)  | 40 (9%)  | 8           | 26  |
| 57  | B3    | 211/211 (100%)    | 191 (90%)  | 20 (10%) | 8           | 25  |
| 58  | C3    | 226/226 (100%)    | 199 (88%)  | 27 (12%) | 5           | 18  |
| 59  | D3    | 128/148 (86%)     | 117 (91%)  | 11 (9%)  | 10          | 29  |
| 60  | E3    | 95/123 (77%)      | 89 (94%)   | 6 (6%)   | 16          | 37  |
| 61  | F3    | 81/103 (79%)      | 73 (90%)   | 8 (10%)  | 7           | 24  |
| 62  | G3    | 68/79 (86%)       | 52 (76%)   | 16 (24%) | 1           | 5   |
| 63  | H3    | 67/76 (88%)       | 58 (87%)   | 9 (13%)  | 4           | 14  |
| 64  | I3    | 58/59 (98%)       | 51 (88%)   | 7 (12%)  | 5           | 17  |
| 65  | J3    | 47/68 (69%)       | 41 (87%)   | 6 (13%)  | 4           | 15  |
| 66  | K3    | 39/66 (59%)       | 36 (92%)   | 3 (8%)   | 12          | 32  |
| 67  | L3    | 40/55 (73%)       | 37 (92%)   | 3 (8%)   | 12          | 33  |
| 68  | M3    | 37/57 (65%)       | 34 (92%)   | 3 (8%)   | 11          | 31  |
| All | All   | 10651/12921 (82%) | 9696 (91%) | 955 (9%) | 11          | 27  |

All (955) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 3   | THR  |
| 1   | A1    | 13  | GLU  |
| 1   | A1    | 24  | ARG  |
| 1   | A1    | 31  | SER  |
| 1   | A1    | 35  | CYS  |
| 1   | A1    | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 42  | ASP  |
| 1   | A1    | 46  | ARG  |
| 1   | A1    | 48  | GLU  |
| 1   | A1    | 49  | SER  |
| 1   | A1    | 65  | LYS  |
| 1   | A1    | 68  | LYS  |
| 1   | A1    | 70  | ARG  |
| 1   | A1    | 75  | LEU  |
| 1   | A1    | 79  | VAL  |
| 1   | A1    | 86  | LEU  |
| 1   | A1    | 89  | TYR  |
| 1   | A1    | 90  | SER  |
| 1   | A1    | 91  | THR  |
| 1   | A1    | 92  | ARG  |
| 1   | A1    | 97  | TYR  |
| 1   | A1    | 99  | ILE  |
| 1   | A1    | 102 | LEU  |
| 1   | A1    | 108 | LYS  |
| 1   | A1    | 112 | LEU  |
| 1   | A1    | 120 | CYS  |
| 1   | A1    | 125 | SER  |
| 1   | A1    | 127 | ILE  |
| 1   | A1    | 128 | GLU  |
| 1   | A1    | 130 | GLU  |
| 1   | A1    | 133 | VAL  |
| 1   | A1    | 134 | ILE  |
| 1   | A1    | 138 | LEU  |
| 1   | A1    | 143 | THR  |
| 1   | A1    | 149 | VAL  |
| 1   | A1    | 156 | THR  |
| 1   | A1    | 159 | GLN  |
| 1   | A1    | 163 | LEU  |
| 1   | A1    | 174 | VAL  |
| 1   | A1    | 175 | ARG  |
| 1   | A1    | 176 | LYS  |
| 1   | A1    | 177 | LEU  |
| 1   | A1    | 178 | SER  |
| 1   | A1    | 179 | ARG  |
| 1   | A1    | 183 | THR  |
| 1   | A1    | 187 | SER  |
| 1   | A1    | 191 | LYS  |
| 1   | A1    | 195 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 196 | VAL  |
| 1   | A1    | 197 | LEU  |
| 1   | A1    | 208 | LEU  |
| 1   | A1    | 211 | LEU  |
| 1   | A1    | 213 | GLN  |
| 1   | A1    | 216 | PHE  |
| 1   | A1    | 239 | SER  |
| 1   | A1    | 241 | ILE  |
| 1   | A1    | 245 | GLU  |
| 1   | A1    | 246 | ASP  |
| 1   | A1    | 248 | LEU  |
| 1   | A1    | 255 | ILE  |
| 1   | A1    | 272 | VAL  |
| 1   | A1    | 277 | ILE  |
| 1   | A1    | 296 | SER  |
| 1   | A1    | 302 | LYS  |
| 1   | A1    | 312 | ILE  |
| 1   | A1    | 316 | ASP  |
| 1   | A1    | 330 | SER  |
| 1   | A1    | 334 | MET  |
| 1   | A1    | 337 | VAL  |
| 1   | A1    | 341 | GLN  |
| 1   | A1    | 344 | ARG  |
| 1   | A1    | 346 | CYS  |
| 1   | A1    | 351 | GLU  |
| 1   | A1    | 352 | SER  |
| 1   | A1    | 353 | GLU  |
| 1   | A1    | 356 | ARG  |
| 1   | A1    | 358 | LYS  |
| 1   | A1    | 360 | LEU  |
| 1   | A1    | 366 | VAL  |
| 1   | A1    | 367 | SER  |
| 1   | A1    | 370 | ASP  |
| 1   | A1    | 379 | ILE  |
| 1   | A1    | 384 | LEU  |
| 1   | A1    | 386 | TYR  |
| 1   | A1    | 398 | ARG  |
| 1   | A1    | 407 | VAL  |
| 1   | A1    | 413 | LYS  |
| 1   | A1    | 428 | ILE  |
| 1   | A1    | 441 | MET  |
| 2   | B1    | 23  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B1    | 24  | LEU  |
| 2   | B1    | 35  | ILE  |
| 2   | B1    | 37  | SER  |
| 2   | B1    | 38  | LEU  |
| 2   | B1    | 45  | SER  |
| 2   | B1    | 46  | ARG  |
| 2   | B1    | 51  | ILE  |
| 2   | B1    | 52  | LYS  |
| 2   | B1    | 56  | ARG  |
| 2   | B1    | 58  | GLU  |
| 2   | B1    | 60  | SER  |
| 2   | B1    | 74  | SER  |
| 2   | B1    | 77  | THR  |
| 2   | B1    | 78  | LYS  |
| 2   | B1    | 81  | SER  |
| 2   | B1    | 85  | ILE  |
| 2   | B1    | 86  | THR  |
| 2   | B1    | 95  | LYS  |
| 2   | B1    | 96  | LEU  |
| 2   | B1    | 99  | THR  |
| 2   | B1    | 101 | THR  |
| 2   | B1    | 108 | THR  |
| 2   | B1    | 112 | LEU  |
| 2   | B1    | 113 | ARG  |
| 2   | B1    | 117 | ASP  |
| 2   | B1    | 119 | LEU  |
| 2   | B1    | 131 | GLU  |
| 2   | B1    | 134 | ARG  |
| 2   | B1    | 140 | LEU  |
| 2   | B1    | 145 | ARG  |
| 2   | B1    | 159 | VAL  |
| 2   | B1    | 160 | ILE  |
| 2   | B1    | 175 | SER  |
| 2   | B1    | 185 | LYS  |
| 2   | B1    | 187 | THR  |
| 2   | B1    | 190 | GLU  |
| 2   | B1    | 196 | GLN  |
| 2   | B1    | 203 | ARG  |
| 2   | B1    | 206 | LEU  |
| 2   | B1    | 215 | VAL  |
| 2   | B1    | 219 | VAL  |
| 2   | B1    | 238 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B1    | 240 | HIS  |
| 2   | B1    | 245 | ARG  |
| 2   | B1    | 253 | VAL  |
| 2   | B1    | 264 | ILE  |
| 2   | B1    | 286 | LYS  |
| 2   | B1    | 292 | THR  |
| 2   | B1    | 294 | SER  |
| 2   | B1    | 295 | LEU  |
| 2   | B1    | 297 | GLN  |
| 2   | B1    | 310 | SER  |
| 2   | B1    | 318 | ASP  |
| 2   | B1    | 319 | SER  |
| 2   | B1    | 327 | ILE  |
| 2   | B1    | 328 | SER  |
| 2   | B1    | 337 | ILE  |
| 2   | B1    | 347 | ILE  |
| 2   | B1    | 353 | SER  |
| 2   | B1    | 354 | ASN  |
| 2   | B1    | 374 | SER  |
| 2   | B1    | 391 | SER  |
| 2   | B1    | 393 | THR  |
| 2   | B1    | 396 | SER  |
| 2   | B1    | 402 | ILE  |
| 2   | B1    | 416 | LYS  |
| 2   | B1    | 418 | VAL  |
| 2   | B1    | 422 | LYS  |
| 2   | B1    | 423 | SER  |
| 2   | B1    | 430 | LEU  |
| 2   | B1    | 436 | ILE  |
| 2   | B1    | 437 | ASP  |
| 2   | B1    | 438 | GLU  |
| 3   | C1    | 1   | MET  |
| 3   | C1    | 5   | ARG  |
| 3   | C1    | 6   | LYS  |
| 3   | C1    | 7   | SER  |
| 3   | C1    | 11  | MET  |
| 3   | C1    | 25  | SER  |
| 3   | C1    | 26  | ASN  |
| 3   | C1    | 27  | ILE  |
| 3   | C1    | 29  | SER  |
| 3   | C1    | 32  | ASN  |
| 3   | C1    | 39  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C1    | 43  | LEU  |
| 3   | C1    | 51  | LEU  |
| 3   | C1    | 57  | SER  |
| 3   | C1    | 60  | THR  |
| 3   | C1    | 61  | THR  |
| 3   | C1    | 65  | SER  |
| 3   | C1    | 67  | THR  |
| 3   | C1    | 73  | VAL  |
| 3   | C1    | 78  | ILE  |
| 3   | C1    | 94  | LEU  |
| 3   | C1    | 115 | ILE  |
| 3   | C1    | 118 | ILE  |
| 3   | C1    | 119 | LEU  |
| 3   | C1    | 123 | VAL  |
| 3   | C1    | 138 | MET  |
| 3   | C1    | 139 | SER  |
| 3   | C1    | 144 | THR  |
| 3   | C1    | 156 | ILE  |
| 3   | C1    | 158 | THR  |
| 3   | C1    | 161 | VAL  |
| 3   | C1    | 169 | SER  |
| 3   | C1    | 174 | THR  |
| 3   | C1    | 176 | THR  |
| 3   | C1    | 177 | ARG  |
| 3   | C1    | 188 | ILE  |
| 3   | C1    | 192 | ILE  |
| 3   | C1    | 197 | LEU  |
| 3   | C1    | 198 | LEU  |
| 3   | C1    | 205 | SER  |
| 3   | C1    | 212 | SER  |
| 3   | C1    | 217 | LYS  |
| 3   | C1    | 226 | ILE  |
| 3   | C1    | 229 | ILE  |
| 3   | C1    | 233 | LEU  |
| 3   | C1    | 237 | LEU  |
| 3   | C1    | 240 | MET  |
| 3   | C1    | 241 | LEU  |
| 3   | C1    | 243 | VAL  |
| 3   | C1    | 244 | LEU  |
| 3   | C1    | 247 | PRO  |
| 3   | C1    | 262 | LEU  |
| 3   | C1    | 271 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C1    | 273 | TYR  |
| 3   | C1    | 280 | ILE  |
| 3   | C1    | 281 | LEU  |
| 3   | C1    | 282 | ARG  |
| 3   | C1    | 284 | ILE  |
| 3   | C1    | 291 | VAL  |
| 3   | C1    | 299 | LEU  |
| 3   | C1    | 304 | ILE  |
| 3   | C1    | 310 | SER  |
| 3   | C1    | 311 | LYS  |
| 3   | C1    | 312 | GLN  |
| 3   | C1    | 313 | ARG  |
| 3   | C1    | 314 | SER  |
| 3   | C1    | 316 | MET  |
| 3   | C1    | 318 | ARG  |
| 3   | C1    | 321 | SER  |
| 3   | C1    | 324 | LEU  |
| 3   | C1    | 343 | VAL  |
| 3   | C1    | 353 | LEU  |
| 3   | C1    | 362 | ILE  |
| 3   | C1    | 363 | LEU  |
| 3   | C1    | 375 | LYS  |
| 3   | C1    | 377 | LEU  |
| 4   | D1    | 3   | LEU  |
| 4   | D1    | 9   | SER  |
| 4   | D1    | 10  | TYR  |
| 4   | D1    | 17  | LEU  |
| 4   | D1    | 20  | SER  |
| 4   | D1    | 21  | LEU  |
| 4   | D1    | 26  | ILE  |
| 4   | D1    | 27  | ARG  |
| 4   | D1    | 32  | VAL  |
| 4   | D1    | 40  | CYS  |
| 4   | D1    | 42  | SER  |
| 4   | D1    | 43  | MET  |
| 4   | D1    | 52  | VAL  |
| 4   | D1    | 55  | CYS  |
| 4   | D1    | 80  | MET  |
| 4   | D1    | 82  | MET  |
| 4   | D1    | 83  | ARG  |
| 4   | D1    | 87  | LEU  |
| 4   | D1    | 106 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D1    | 116 | ILE  |
| 4   | D1    | 120 | ARG  |
| 4   | D1    | 124 | GLU  |
| 4   | D1    | 127 | VAL  |
| 4   | D1    | 132 | THR  |
| 4   | D1    | 139 | THR  |
| 4   | D1    | 141 | VAL  |
| 4   | D1    | 179 | MET  |
| 4   | D1    | 182 | VAL  |
| 4   | D1    | 186 | VAL  |
| 4   | D1    | 201 | ARG  |
| 4   | D1    | 208 | MET  |
| 4   | D1    | 218 | LEU  |
| 4   | D1    | 228 | SER  |
| 4   | D1    | 231 | LYS  |
| 5   | E1    | 1   | SER  |
| 5   | E1    | 5   | ILE  |
| 5   | E1    | 6   | LYS  |
| 5   | E1    | 11  | SER  |
| 5   | E1    | 14  | ARG  |
| 5   | E1    | 15  | ARG  |
| 5   | E1    | 17  | GLU  |
| 5   | E1    | 19  | LEU  |
| 5   | E1    | 28  | SER  |
| 5   | E1    | 30  | GLU  |
| 5   | E1    | 32  | ARG  |
| 5   | E1    | 33  | LYS  |
| 5   | E1    | 40  | THR  |
| 5   | E1    | 52  | LYS  |
| 5   | E1    | 58  | PHE  |
| 5   | E1    | 63  | SER  |
| 5   | E1    | 67  | ASP  |
| 5   | E1    | 68  | VAL  |
| 6   | F1    | 7   | SER  |
| 6   | F1    | 9   | SER  |
| 6   | F1    | 10  | SER  |
| 6   | F1    | 11  | ARG  |
| 6   | F1    | 13  | LEU  |
| 6   | F1    | 16  | ILE  |
| 6   | F1    | 18  | LYS  |
| 6   | F1    | 35  | ASP  |
| 6   | F1    | 44  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F1    | 47  | ILE  |
| 6   | F1    | 48  | ARG  |
| 6   | F1    | 50  | LEU  |
| 6   | F1    | 53  | ASN  |
| 6   | F1    | 54  | LEU  |
| 6   | F1    | 58  | ARG  |
| 6   | F1    | 68  | LEU  |
| 6   | F1    | 69  | SER  |
| 6   | F1    | 70  | MET  |
| 6   | F1    | 74  | ILE  |
| 6   | F1    | 77  | LYS  |
| 6   | F1    | 82  | LYS  |
| 6   | F1    | 88  | SER  |
| 6   | F1    | 90  | LEU  |
| 6   | F1    | 94  | LEU  |
| 6   | F1    | 95  | LYS  |
| 6   | F1    | 98  | ILE  |
| 6   | F1    | 100 | GLU  |
| 6   | F1    | 110 | LYS  |
| 7   | G1    | 4   | PHE  |
| 7   | G1    | 8   | THR  |
| 7   | G1    | 9   | ARG  |
| 7   | G1    | 10  | VAL  |
| 7   | G1    | 15  | THR  |
| 7   | G1    | 19  | SER  |
| 7   | G1    | 23  | GLN  |
| 7   | G1    | 24  | ARG  |
| 7   | G1    | 39  | ARG  |
| 7   | G1    | 40  | ARG  |
| 7   | G1    | 41  | THR  |
| 7   | G1    | 42  | ARG  |
| 7   | G1    | 45  | ILE  |
| 7   | G1    | 46  | LEU  |
| 7   | G1    | 58  | VAL  |
| 7   | G1    | 60  | THR  |
| 7   | G1    | 69  | SER  |
| 7   | G1    | 70  | LYS  |
| 8   | H1    | 20  | VAL  |
| 8   | H1    | 29  | LYS  |
| 8   | H1    | 30  | CYS  |
| 8   | H1    | 31  | VAL  |
| 8   | H1    | 54  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H1    | 57  | GLU  |
| 8   | H1    | 58  | LEU  |
| 8   | H1    | 59  | LEU  |
| 8   | H1    | 73  | LEU  |
| 8   | H1    | 74  | PHE  |
| 8   | H1    | 76  | SER  |
| 9   | I1    | 46  | LYS  |
| 9   | I1    | 49  | VAL  |
| 9   | I1    | 54  | SER  |
| 9   | I1    | 69  | SER  |
| 9   | I1    | 70  | LEU  |
| 9   | I1    | 72  | VAL  |
| 9   | I1    | 76  | VAL  |
| 9   | I1    | 77  | ARG  |
| 9   | I1    | 78  | TYR  |
| 10  | J1    | 4   | THR  |
| 10  | J1    | 11  | SER  |
| 10  | J1    | 13  | LEU  |
| 10  | J1    | 17  | THR  |
| 10  | J1    | 18  | SER  |
| 10  | J1    | 24  | ILE  |
| 10  | J1    | 25  | VAL  |
| 10  | J1    | 46  | ILE  |
| 10  | J1    | 58  | LYS  |
| 11  | K1    | 20  | THR  |
| 11  | K1    | 23  | LEU  |
| 11  | K1    | 27  | VAL  |
| 11  | K1    | 36  | THR  |
| 1   | M1    | 3   | THR  |
| 1   | M1    | 13  | GLU  |
| 1   | M1    | 24  | ARG  |
| 1   | M1    | 31  | SER  |
| 1   | M1    | 37  | VAL  |
| 1   | M1    | 42  | ASP  |
| 1   | M1    | 45  | SER  |
| 1   | M1    | 46  | ARG  |
| 1   | M1    | 48  | GLU  |
| 1   | M1    | 51  | LYS  |
| 1   | M1    | 70  | ARG  |
| 1   | M1    | 79  | VAL  |
| 1   | M1    | 86  | LEU  |
| 1   | M1    | 89  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M1    | 91  | THR  |
| 1   | M1    | 92  | ARG  |
| 1   | M1    | 97  | TYR  |
| 1   | M1    | 99  | ILE  |
| 1   | M1    | 108 | LYS  |
| 1   | M1    | 112 | LEU  |
| 1   | M1    | 125 | SER  |
| 1   | M1    | 127 | ILE  |
| 1   | M1    | 128 | GLU  |
| 1   | M1    | 130 | GLU  |
| 1   | M1    | 133 | VAL  |
| 1   | M1    | 137 | GLU  |
| 1   | M1    | 138 | LEU  |
| 1   | M1    | 143 | THR  |
| 1   | M1    | 149 | VAL  |
| 1   | M1    | 156 | THR  |
| 1   | M1    | 159 | GLN  |
| 1   | M1    | 163 | LEU  |
| 1   | M1    | 174 | VAL  |
| 1   | M1    | 175 | ARG  |
| 1   | M1    | 176 | LYS  |
| 1   | M1    | 177 | LEU  |
| 1   | M1    | 179 | ARG  |
| 1   | M1    | 183 | THR  |
| 1   | M1    | 187 | SER  |
| 1   | M1    | 191 | LYS  |
| 1   | M1    | 195 | MET  |
| 1   | M1    | 197 | LEU  |
| 1   | M1    | 208 | LEU  |
| 1   | M1    | 211 | LEU  |
| 1   | M1    | 213 | GLN  |
| 1   | M1    | 216 | PHE  |
| 1   | M1    | 245 | GLU  |
| 1   | M1    | 246 | ASP  |
| 1   | M1    | 248 | LEU  |
| 1   | M1    | 257 | VAL  |
| 1   | M1    | 277 | ILE  |
| 1   | M1    | 296 | SER  |
| 1   | M1    | 302 | LYS  |
| 1   | M1    | 307 | PHE  |
| 1   | M1    | 309 | THR  |
| 1   | M1    | 316 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M1    | 319 | LEU  |
| 1   | M1    | 329 | MET  |
| 1   | M1    | 330 | SER  |
| 1   | M1    | 334 | MET  |
| 1   | M1    | 337 | VAL  |
| 1   | M1    | 341 | GLN  |
| 1   | M1    | 344 | ARG  |
| 1   | M1    | 346 | CYS  |
| 1   | M1    | 347 | THR  |
| 1   | M1    | 351 | GLU  |
| 1   | M1    | 353 | GLU  |
| 1   | M1    | 356 | ARG  |
| 1   | M1    | 358 | LYS  |
| 1   | M1    | 360 | LEU  |
| 1   | M1    | 366 | VAL  |
| 1   | M1    | 370 | ASP  |
| 1   | M1    | 379 | ILE  |
| 1   | M1    | 382 | SER  |
| 1   | M1    | 384 | LEU  |
| 1   | M1    | 386 | TYR  |
| 1   | M1    | 407 | VAL  |
| 1   | M1    | 412 | SER  |
| 1   | M1    | 413 | LYS  |
| 1   | M1    | 419 | CYS  |
| 1   | M1    | 428 | ILE  |
| 1   | M1    | 441 | MET  |
| 2   | N1    | 23  | ASP  |
| 2   | N1    | 24  | LEU  |
| 2   | N1    | 35  | ILE  |
| 2   | N1    | 37  | SER  |
| 2   | N1    | 38  | LEU  |
| 2   | N1    | 45  | SER  |
| 2   | N1    | 46  | ARG  |
| 2   | N1    | 52  | LYS  |
| 2   | N1    | 56  | ARG  |
| 2   | N1    | 58  | GLU  |
| 2   | N1    | 60  | SER  |
| 2   | N1    | 65  | THR  |
| 2   | N1    | 78  | LYS  |
| 2   | N1    | 81  | SER  |
| 2   | N1    | 84  | LYS  |
| 2   | N1    | 85  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N1    | 86  | THR  |
| 2   | N1    | 96  | LEU  |
| 2   | N1    | 99  | THR  |
| 2   | N1    | 100 | SER  |
| 2   | N1    | 101 | THR  |
| 2   | N1    | 102 | ARG  |
| 2   | N1    | 108 | THR  |
| 2   | N1    | 111 | CYS  |
| 2   | N1    | 112 | LEU  |
| 2   | N1    | 113 | ARG  |
| 2   | N1    | 117 | ASP  |
| 2   | N1    | 119 | LEU  |
| 2   | N1    | 134 | ARG  |
| 2   | N1    | 145 | ARG  |
| 2   | N1    | 159 | VAL  |
| 2   | N1    | 160 | ILE  |
| 2   | N1    | 175 | SER  |
| 2   | N1    | 183 | ILE  |
| 2   | N1    | 185 | LYS  |
| 2   | N1    | 190 | GLU  |
| 2   | N1    | 196 | GLN  |
| 2   | N1    | 201 | SER  |
| 2   | N1    | 203 | ARG  |
| 2   | N1    | 206 | LEU  |
| 2   | N1    | 207 | ILE  |
| 2   | N1    | 215 | VAL  |
| 2   | N1    | 219 | VAL  |
| 2   | N1    | 233 | SER  |
| 2   | N1    | 238 | LYS  |
| 2   | N1    | 240 | HIS  |
| 2   | N1    | 244 | ILE  |
| 2   | N1    | 253 | VAL  |
| 2   | N1    | 264 | ILE  |
| 2   | N1    | 266 | SER  |
| 2   | N1    | 286 | LYS  |
| 2   | N1    | 292 | THR  |
| 2   | N1    | 295 | LEU  |
| 2   | N1    | 297 | GLN  |
| 2   | N1    | 315 | SER  |
| 2   | N1    | 317 | SER  |
| 2   | N1    | 318 | ASP  |
| 2   | N1    | 327 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N1    | 328 | SER  |
| 2   | N1    | 329 | GLN  |
| 2   | N1    | 337 | ILE  |
| 2   | N1    | 345 | LYS  |
| 2   | N1    | 346 | THR  |
| 2   | N1    | 354 | ASN  |
| 2   | N1    | 357 | VAL  |
| 2   | N1    | 384 | SER  |
| 2   | N1    | 402 | ILE  |
| 2   | N1    | 403 | ASP  |
| 2   | N1    | 416 | LYS  |
| 2   | N1    | 418 | VAL  |
| 2   | N1    | 424 | MET  |
| 2   | N1    | 436 | ILE  |
| 2   | N1    | 437 | ASP  |
| 2   | N1    | 438 | GLU  |
| 3   | O1    | 1   | MET  |
| 3   | O1    | 5   | ARG  |
| 3   | O1    | 6   | LYS  |
| 3   | O1    | 7   | SER  |
| 3   | O1    | 11  | MET  |
| 3   | O1    | 13  | ILE  |
| 3   | O1    | 27  | ILE  |
| 3   | O1    | 32  | ASN  |
| 3   | O1    | 35  | SER  |
| 3   | O1    | 39  | ILE  |
| 3   | O1    | 44  | GLN  |
| 3   | O1    | 60  | THR  |
| 3   | O1    | 61  | THR  |
| 3   | O1    | 67  | THR  |
| 3   | O1    | 69  | ILE  |
| 3   | O1    | 73  | VAL  |
| 3   | O1    | 92  | ILE  |
| 3   | O1    | 94  | LEU  |
| 3   | O1    | 100 | ARG  |
| 3   | O1    | 115 | ILE  |
| 3   | O1    | 118 | ILE  |
| 3   | O1    | 119 | LEU  |
| 3   | O1    | 138 | MET  |
| 3   | O1    | 139 | SER  |
| 3   | O1    | 144 | THR  |
| 3   | O1    | 153 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | O1    | 156 | ILE  |
| 3   | O1    | 158 | THR  |
| 3   | O1    | 161 | VAL  |
| 3   | O1    | 169 | SER  |
| 3   | O1    | 174 | THR  |
| 3   | O1    | 176 | THR  |
| 3   | O1    | 184 | ILE  |
| 3   | O1    | 188 | ILE  |
| 3   | O1    | 189 | ILE  |
| 3   | O1    | 192 | ILE  |
| 3   | O1    | 197 | LEU  |
| 3   | O1    | 212 | SER  |
| 3   | O1    | 215 | VAL  |
| 3   | O1    | 226 | ILE  |
| 3   | O1    | 229 | ILE  |
| 3   | O1    | 233 | LEU  |
| 3   | O1    | 241 | LEU  |
| 3   | O1    | 242 | LEU  |
| 3   | O1    | 243 | VAL  |
| 3   | O1    | 244 | LEU  |
| 3   | O1    | 257 | THR  |
| 3   | O1    | 262 | LEU  |
| 3   | O1    | 271 | GLU  |
| 3   | O1    | 281 | LEU  |
| 3   | O1    | 282 | ARG  |
| 3   | O1    | 287 | LYS  |
| 3   | O1    | 291 | VAL  |
| 3   | O1    | 297 | SER  |
| 3   | O1    | 299 | LEU  |
| 3   | O1    | 300 | ILE  |
| 3   | O1    | 313 | ARG  |
| 3   | O1    | 316 | MET  |
| 3   | O1    | 318 | ARG  |
| 3   | O1    | 324 | LEU  |
| 3   | O1    | 338 | ILE  |
| 3   | O1    | 349 | THR  |
| 3   | O1    | 356 | VAL  |
| 3   | O1    | 362 | ILE  |
| 3   | O1    | 363 | LEU  |
| 3   | O1    | 375 | LYS  |
| 3   | O1    | 377 | LEU  |
| 3   | O1    | 378 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | P1    | 3   | LEU  |
| 4   | P1    | 10  | TYR  |
| 4   | P1    | 13  | SER  |
| 4   | P1    | 17  | LEU  |
| 4   | P1    | 20  | SER  |
| 4   | P1    | 21  | LEU  |
| 4   | P1    | 38  | SER  |
| 4   | P1    | 39  | SER  |
| 4   | P1    | 40  | CYS  |
| 4   | P1    | 42  | SER  |
| 4   | P1    | 43  | MET  |
| 4   | P1    | 52  | VAL  |
| 4   | P1    | 55  | CYS  |
| 4   | P1    | 80  | MET  |
| 4   | P1    | 82  | MET  |
| 4   | P1    | 83  | ARG  |
| 4   | P1    | 88  | SER  |
| 4   | P1    | 106 | ASN  |
| 4   | P1    | 120 | ARG  |
| 4   | P1    | 124 | GLU  |
| 4   | P1    | 127 | VAL  |
| 4   | P1    | 132 | THR  |
| 4   | P1    | 139 | THR  |
| 4   | P1    | 141 | VAL  |
| 4   | P1    | 158 | ILE  |
| 4   | P1    | 160 | MET  |
| 4   | P1    | 179 | MET  |
| 4   | P1    | 180 | SER  |
| 4   | P1    | 182 | VAL  |
| 4   | P1    | 186 | VAL  |
| 4   | P1    | 201 | ARG  |
| 4   | P1    | 208 | MET  |
| 4   | P1    | 210 | LEU  |
| 4   | P1    | 223 | LYS  |
| 4   | P1    | 226 | LYS  |
| 4   | P1    | 231 | LYS  |
| 5   | Q1    | 5   | ILE  |
| 5   | Q1    | 6   | LYS  |
| 5   | Q1    | 11  | SER  |
| 5   | Q1    | 14  | ARG  |
| 5   | Q1    | 17  | GLU  |
| 5   | Q1    | 18  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Q1    | 19  | LEU  |
| 5   | Q1    | 22  | THR  |
| 5   | Q1    | 23  | LYS  |
| 5   | Q1    | 28  | SER  |
| 5   | Q1    | 30  | GLU  |
| 5   | Q1    | 32  | ARG  |
| 5   | Q1    | 33  | LYS  |
| 5   | Q1    | 36  | SER  |
| 5   | Q1    | 40  | THR  |
| 5   | Q1    | 42  | THR  |
| 5   | Q1    | 43  | THR  |
| 5   | Q1    | 44  | THR  |
| 5   | Q1    | 45  | VAL  |
| 5   | Q1    | 58  | PHE  |
| 5   | Q1    | 60  | SER  |
| 5   | Q1    | 61  | SER  |
| 5   | Q1    | 62  | MET  |
| 5   | Q1    | 63  | SER  |
| 5   | Q1    | 65  | SER  |
| 5   | Q1    | 68  | VAL  |
| 5   | Q1    | 71  | MET  |
| 5   | Q1    | 73  | LYS  |
| 5   | Q1    | 74  | ILE  |
| 5   | Q1    | 76  | ILE  |
| 5   | Q1    | 78  | LEU  |
| 5   | Q1    | 81  | ILE  |
| 5   | Q1    | 87  | MET  |
| 5   | Q1    | 95  | PRO  |
| 5   | Q1    | 98  | VAL  |
| 5   | Q1    | 102 | THR  |
| 5   | Q1    | 103 | LYS  |
| 5   | Q1    | 106 | ILE  |
| 5   | Q1    | 109 | GLU  |
| 5   | Q1    | 113 | GLU  |
| 5   | Q1    | 114 | VAL  |
| 5   | Q1    | 125 | GLU  |
| 5   | Q1    | 129 | LYS  |
| 5   | Q1    | 136 | ILE  |
| 5   | Q1    | 139 | CYS  |
| 5   | Q1    | 140 | THR  |
| 5   | Q1    | 144 | CYS  |
| 5   | Q1    | 147 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Q1    | 152 | ASP  |
| 5   | Q1    | 158 | CYS  |
| 5   | Q1    | 168 | SER  |
| 5   | Q1    | 171 | ILE  |
| 5   | Q1    | 172 | ARG  |
| 5   | Q1    | 178 | LEU  |
| 5   | Q1    | 192 | MET  |
| 5   | Q1    | 194 | ILE  |
| 5   | Q1    | 195 | VAL  |
| 6   | R1    | 7   | SER  |
| 6   | R1    | 11  | ARG  |
| 6   | R1    | 16  | ILE  |
| 6   | R1    | 35  | ASP  |
| 6   | R1    | 47  | ILE  |
| 6   | R1    | 48  | ARG  |
| 6   | R1    | 54  | LEU  |
| 6   | R1    | 64  | ARG  |
| 6   | R1    | 68  | LEU  |
| 6   | R1    | 70  | MET  |
| 6   | R1    | 75  | LEU  |
| 6   | R1    | 77  | LYS  |
| 6   | R1    | 88  | SER  |
| 6   | R1    | 90  | LEU  |
| 6   | R1    | 94  | LEU  |
| 6   | R1    | 98  | ILE  |
| 6   | R1    | 100 | GLU  |
| 6   | R1    | 101 | ARG  |
| 6   | R1    | 103 | GLU  |
| 6   | R1    | 110 | LYS  |
| 7   | S1    | 4   | PHE  |
| 7   | S1    | 7   | LEU  |
| 7   | S1    | 8   | THR  |
| 7   | S1    | 9   | ARG  |
| 7   | S1    | 10  | VAL  |
| 7   | S1    | 15  | THR  |
| 7   | S1    | 18  | LEU  |
| 7   | S1    | 19  | SER  |
| 7   | S1    | 23  | GLN  |
| 7   | S1    | 24  | ARG  |
| 7   | S1    | 31  | SER  |
| 7   | S1    | 39  | ARG  |
| 7   | S1    | 40  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | S1    | 41  | THR  |
| 7   | S1    | 42  | ARG  |
| 7   | S1    | 45  | ILE  |
| 7   | S1    | 46  | LEU  |
| 7   | S1    | 58  | VAL  |
| 7   | S1    | 69  | SER  |
| 7   | S1    | 70  | LYS  |
| 8   | T1    | 20  | VAL  |
| 8   | T1    | 29  | LYS  |
| 8   | T1    | 30  | CYS  |
| 8   | T1    | 31  | VAL  |
| 8   | T1    | 46  | SER  |
| 8   | T1    | 48  | SER  |
| 8   | T1    | 54  | CYS  |
| 8   | T1    | 57  | GLU  |
| 8   | T1    | 58  | LEU  |
| 8   | T1    | 73  | LEU  |
| 8   | T1    | 74  | PHE  |
| 9   | U1    | 46  | LYS  |
| 9   | U1    | 49  | VAL  |
| 9   | U1    | 68  | VAL  |
| 9   | U1    | 70  | LEU  |
| 9   | U1    | 72  | VAL  |
| 9   | U1    | 76  | VAL  |
| 9   | U1    | 77  | ARG  |
| 9   | U1    | 78  | TYR  |
| 10  | V1    | 4   | THR  |
| 10  | V1    | 9   | LEU  |
| 10  | V1    | 12  | LEU  |
| 10  | V1    | 13  | LEU  |
| 10  | V1    | 16  | ARG  |
| 10  | V1    | 18  | SER  |
| 10  | V1    | 42  | ILE  |
| 10  | V1    | 46  | ILE  |
| 10  | V1    | 55  | ILE  |
| 10  | V1    | 58  | LYS  |
| 11  | W1    | 20  | THR  |
| 11  | W1    | 23  | LEU  |
| 11  | W1    | 27  | VAL  |
| 11  | W1    | 33  | VAL  |
| 11  | W1    | 36  | THR  |
| 18  | 92    | 93  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | A2    | 253 | VAL  |
| 19  | A2    | 341 | ILE  |
| 19  | A2    | 538 | GLN  |
| 20  | B2    | 92  | HIS  |
| 20  | B2    | 94  | VAL  |
| 20  | B2    | 95  | LEU  |
| 20  | B2    | 96  | ARG  |
| 20  | B2    | 97  | LEU  |
| 20  | B2    | 372 | LYS  |
| 21  | C2    | 218 | VAL  |
| 22  | D2    | 113 | PHE  |
| 22  | D2    | 114 | ARG  |
| 22  | D2    | 181 | ILE  |
| 23  | E2    | 77  | LEU  |
| 27  | I2    | 101 | ILE  |
| 27  | I2    | 103 | LEU  |
| 27  | I2    | 105 | LYS  |
| 27  | I2    | 106 | GLU  |
| 34  | Q2    | 115 | LEU  |
| 34  | Q2    | 128 | VAL  |
| 35  | R2    | 152 | ILE  |
| 36  | S2    | 200 | PRO  |
| 36  | S2    | 216 | LYS  |
| 44  | a2    | 76  | ILE  |
| 52  | 12    | 25  | ARG  |
| 52  | 12    | 126 | LYS  |
| 52  | 12    | 134 | ARG  |
| 52  | 12    | 187 | ILE  |
| 52  | 12    | 224 | PHE  |
| 52  | 12    | 228 | TYR  |
| 52  | 12    | 240 | ILE  |
| 52  | 12    | 310 | LEU  |
| 53  | 62    | 427 | ILE  |
| 55  | e2    | 75  | TYR  |
| 56  | A3    | 18  | LEU  |
| 56  | A3    | 35  | LEU  |
| 56  | A3    | 92  | MET  |
| 56  | A3    | 96  | ARG  |
| 56  | A3    | 105 | LEU  |
| 56  | A3    | 115 | SER  |
| 56  | A3    | 136 | LEU  |
| 56  | A3    | 138 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | A3    | 150 | LEU  |
| 56  | A3    | 158 | ILE  |
| 56  | A3    | 159 | LEU  |
| 56  | A3    | 187 | SER  |
| 56  | A3    | 188 | VAL  |
| 56  | A3    | 189 | MET  |
| 56  | A3    | 194 | LEU  |
| 56  | A3    | 199 | LEU  |
| 56  | A3    | 213 | ARG  |
| 56  | A3    | 241 | PRO  |
| 56  | A3    | 273 | MET  |
| 56  | A3    | 295 | VAL  |
| 56  | A3    | 301 | THR  |
| 56  | A3    | 306 | THR  |
| 56  | A3    | 318 | VAL  |
| 56  | A3    | 324 | LEU  |
| 56  | A3    | 347 | LEU  |
| 56  | A3    | 353 | LEU  |
| 56  | A3    | 354 | THR  |
| 56  | A3    | 365 | ILE  |
| 56  | A3    | 369 | ASP  |
| 56  | A3    | 373 | VAL  |
| 56  | A3    | 383 | MET  |
| 56  | A3    | 417 | MET  |
| 56  | A3    | 444 | PRO  |
| 56  | A3    | 465 | VAL  |
| 56  | A3    | 467 | LEU  |
| 56  | A3    | 474 | GLU  |
| 56  | A3    | 492 | LEU  |
| 56  | A3    | 508 | PRO  |
| 56  | A3    | 509 | THR  |
| 56  | A3    | 512 | ASN  |
| 57  | B3    | 7   | LEU  |
| 57  | B3    | 16  | ILE  |
| 57  | B3    | 31  | VAL  |
| 57  | B3    | 33  | LEU  |
| 57  | B3    | 52  | HIS  |
| 57  | B3    | 60  | GLU  |
| 57  | B3    | 63  | THR  |
| 57  | B3    | 67  | ILE  |
| 57  | B3    | 88  | ASP  |
| 57  | B3    | 92  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | B3    | 125 | THR  |
| 57  | B3    | 130 | PRO  |
| 57  | B3    | 134 | ARG  |
| 57  | B3    | 142 | VAL  |
| 57  | B3    | 147 | GLU  |
| 57  | B3    | 170 | LEU  |
| 57  | B3    | 171 | LYS  |
| 57  | B3    | 185 | MET  |
| 57  | B3    | 205 | SER  |
| 57  | B3    | 216 | LEU  |
| 58  | C3    | 1   | MET  |
| 58  | C3    | 11  | VAL  |
| 58  | C3    | 13  | PRO  |
| 58  | C3    | 14  | SER  |
| 58  | C3    | 18  | LEU  |
| 58  | C3    | 19  | THR  |
| 58  | C3    | 22  | LEU  |
| 58  | C3    | 26  | LEU  |
| 58  | C3    | 38  | ASN  |
| 58  | C3    | 39  | SER  |
| 58  | C3    | 85  | LEU  |
| 58  | C3    | 92  | LEU  |
| 58  | C3    | 112 | LEU  |
| 58  | C3    | 127 | LEU  |
| 58  | C3    | 128 | GLU  |
| 58  | C3    | 131 | LEU  |
| 58  | C3    | 132 | LEU  |
| 58  | C3    | 137 | LEU  |
| 58  | C3    | 142 | VAL  |
| 58  | C3    | 160 | LEU  |
| 58  | C3    | 163 | LEU  |
| 58  | C3    | 188 | ILE  |
| 58  | C3    | 196 | THR  |
| 58  | C3    | 199 | VAL  |
| 58  | C3    | 213 | THR  |
| 58  | C3    | 222 | GLN  |
| 58  | C3    | 230 | ASN  |
| 59  | D3    | 9   | GLU  |
| 59  | D3    | 27  | VAL  |
| 59  | D3    | 31  | LYS  |
| 59  | D3    | 36  | SER  |
| 59  | D3    | 40  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | D3    | 59  | LEU  |
| 59  | D3    | 62  | LEU  |
| 59  | D3    | 107 | ILE  |
| 59  | D3    | 116 | VAL  |
| 59  | D3    | 143 | ASN  |
| 59  | D3    | 147 | LYS  |
| 60  | E3    | 7   | THR  |
| 60  | E3    | 29  | LEU  |
| 60  | E3    | 70  | VAL  |
| 60  | E3    | 79  | LYS  |
| 60  | E3    | 80  | GLU  |
| 60  | E3    | 90  | ARG  |
| 61  | F3    | 6   | VAL  |
| 61  | F3    | 20  | VAL  |
| 61  | F3    | 37  | LYS  |
| 61  | F3    | 52  | ILE  |
| 61  | F3    | 53  | THR  |
| 61  | F3    | 74  | LEU  |
| 61  | F3    | 95  | GLN  |
| 61  | F3    | 98  | HIS  |
| 62  | G3    | 5   | LYS  |
| 62  | G3    | 7   | ASP  |
| 62  | G3    | 8   | HIS  |
| 62  | G3    | 14  | ARG  |
| 62  | G3    | 17  | ARG  |
| 62  | G3    | 33  | LEU  |
| 62  | G3    | 34  | ASN  |
| 62  | G3    | 37  | LEU  |
| 62  | G3    | 41  | HIS  |
| 62  | G3    | 42  | ARG  |
| 62  | G3    | 43  | GLU  |
| 62  | G3    | 48  | ILE  |
| 62  | G3    | 54  | ARG  |
| 62  | G3    | 56  | ARG  |
| 62  | G3    | 68  | THR  |
| 62  | G3    | 78  | LEU  |
| 63  | H3    | 19  | ARG  |
| 63  | H3    | 29  | CYS  |
| 63  | H3    | 41  | LYS  |
| 63  | H3    | 51  | SER  |
| 63  | H3    | 53  | CYS  |
| 63  | H3    | 57  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | H3    | 60  | TYR  |
| 63  | H3    | 67  | SER  |
| 63  | H3    | 75  | ARG  |
| 64  | I3    | 2   | THR  |
| 64  | I3    | 4   | LEU  |
| 64  | I3    | 8   | GLN  |
| 64  | I3    | 22  | VAL  |
| 64  | I3    | 26  | MET  |
| 64  | I3    | 44  | LYS  |
| 64  | I3    | 64  | ARG  |
| 65  | J3    | 2   | GLU  |
| 65  | J3    | 5   | VAL  |
| 65  | J3    | 8   | LYS  |
| 65  | J3    | 16  | ASN  |
| 65  | J3    | 23  | LYS  |
| 65  | J3    | 27  | THR  |
| 66  | K3    | 45  | VAL  |
| 66  | K3    | 48  | VAL  |
| 66  | K3    | 49  | THR  |
| 67  | L3    | 15  | VAL  |
| 67  | L3    | 22  | LEU  |
| 67  | L3    | 26  | THR  |
| 68  | M3    | 13  | LYS  |
| 68  | M3    | 24  | LEU  |
| 68  | M3    | 42  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 18  | GLN  |
| 1   | A1    | 21  | ASN  |
| 1   | A1    | 32  | GLN  |
| 1   | A1    | 73  | ASN  |
| 1   | A1    | 85  | HIS  |
| 1   | A1    | 136 | GLN  |
| 1   | A1    | 151 | ASN  |
| 1   | A1    | 154 | HIS  |
| 1   | A1    | 189 | HIS  |
| 1   | A1    | 240 | GLN  |
| 1   | A1    | 243 | HIS  |
| 1   | A1    | 252 | HIS  |
| 1   | A1    | 289 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 308 | GLN  |
| 1   | A1    | 435 | ASN  |
| 2   | B1    | 62  | ASN  |
| 2   | B1    | 67  | HIS  |
| 2   | B1    | 125 | ASN  |
| 2   | B1    | 162 | ASN  |
| 2   | B1    | 164 | HIS  |
| 2   | B1    | 198 | HIS  |
| 2   | B1    | 247 | GLN  |
| 2   | B1    | 304 | HIS  |
| 2   | B1    | 429 | ASN  |
| 3   | C1    | 15  | ASN  |
| 3   | C1    | 26  | ASN  |
| 3   | C1    | 32  | ASN  |
| 3   | C1    | 114 | ASN  |
| 3   | C1    | 206 | ASN  |
| 3   | C1    | 312 | GLN  |
| 3   | C1    | 374 | ASN  |
| 4   | D1    | 6   | HIS  |
| 4   | D1    | 50  | HIS  |
| 4   | D1    | 75  | ASN  |
| 4   | D1    | 106 | ASN  |
| 4   | D1    | 181 | GLN  |
| 5   | E1    | 57  | GLN  |
| 6   | F1    | 38  | HIS  |
| 7   | G1    | 6   | HIS  |
| 7   | G1    | 36  | ASN  |
| 9   | I1    | 71  | ASN  |
| 10  | J1    | 54  | HIS  |
| 1   | M1    | 18  | GLN  |
| 1   | M1    | 32  | GLN  |
| 1   | M1    | 85  | HIS  |
| 1   | M1    | 136 | GLN  |
| 1   | M1    | 151 | ASN  |
| 1   | M1    | 154 | HIS  |
| 1   | M1    | 159 | GLN  |
| 1   | M1    | 173 | ASN  |
| 1   | M1    | 189 | HIS  |
| 1   | M1    | 213 | GLN  |
| 1   | M1    | 240 | GLN  |
| 1   | M1    | 243 | HIS  |
| 1   | M1    | 308 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M1    | 323 | HIS  |
| 1   | M1    | 339 | GLN  |
| 1   | M1    | 435 | ASN  |
| 2   | N1    | 62  | ASN  |
| 2   | N1    | 67  | HIS  |
| 2   | N1    | 125 | ASN  |
| 2   | N1    | 141 | GLN  |
| 2   | N1    | 198 | HIS  |
| 2   | N1    | 247 | GLN  |
| 2   | N1    | 304 | HIS  |
| 2   | N1    | 429 | ASN  |
| 3   | O1    | 15  | ASN  |
| 3   | O1    | 26  | ASN  |
| 3   | O1    | 32  | ASN  |
| 3   | O1    | 54  | HIS  |
| 3   | O1    | 114 | ASN  |
| 3   | O1    | 206 | ASN  |
| 3   | O1    | 374 | ASN  |
| 4   | P1    | 6   | HIS  |
| 4   | P1    | 50  | HIS  |
| 4   | P1    | 75  | ASN  |
| 4   | P1    | 106 | ASN  |
| 4   | P1    | 181 | GLN  |
| 4   | P1    | 225 | HIS  |
| 5   | Q1    | 53  | ASN  |
| 5   | Q1    | 121 | GLN  |
| 6   | R1    | 38  | HIS  |
| 6   | R1    | 73  | GLN  |
| 7   | S1    | 6   | HIS  |
| 10  | V1    | 54  | HIS  |
| 12  | 22    | 48  | HIS  |
| 12  | 22    | 120 | GLN  |
| 12  | 22    | 186 | HIS  |
| 13  | 32    | 80  | GLN  |
| 14  | 42    | 26  | ASN  |
| 14  | 42    | 83  | HIS  |
| 14  | 42    | 338 | HIS  |
| 14  | 42    | 366 | ASN  |
| 14  | 42    | 374 | ASN  |
| 15  | 52    | 7   | ASN  |
| 16  | 72    | 46  | ASN  |
| 17  | 82    | 220 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | 82    | 346 | GLN  |
| 17  | 82    | 418 | GLN  |
| 17  | 82    | 441 | HIS  |
| 19  | A2    | 140 | GLN  |
| 19  | A2    | 142 | GLN  |
| 19  | A2    | 221 | ASN  |
| 19  | A2    | 359 | ASN  |
| 19  | A2    | 424 | HIS  |
| 19  | A2    | 571 | HIS  |
| 19  | A2    | 572 | HIS  |
| 19  | A2    | 666 | GLN  |
| 20  | B2    | 92  | HIS  |
| 20  | B2    | 131 | GLN  |
| 20  | B2    | 168 | GLN  |
| 20  | B2    | 182 | ASN  |
| 20  | B2    | 250 | ASN  |
| 20  | B2    | 431 | HIS  |
| 21  | C2    | 84  | ASN  |
| 21  | C2    | 140 | ASN  |
| 21  | C2    | 230 | GLN  |
| 22  | D2    | 98  | HIS  |
| 26  | H2    | 27  | HIS  |
| 26  | H2    | 45  | HIS  |
| 26  | H2    | 97  | HIS  |
| 27  | I2    | 102 | ASN  |
| 29  | K2    | 22  | HIS  |
| 29  | K2    | 86  | GLN  |
| 31  | N2    | 83  | GLN  |
| 33  | P2    | 25  | GLN  |
| 34  | Q2    | 103 | GLN  |
| 35  | R2    | 43  | HIS  |
| 35  | R2    | 79  | GLN  |
| 35  | R2    | 84  | HIS  |
| 35  | R2    | 169 | HIS  |
| 35  | R2    | 171 | ASN  |
| 35  | R2    | 251 | ASN  |
| 35  | R2    | 331 | HIS  |
| 36  | S2    | 211 | ASN  |
| 36  | S2    | 223 | GLN  |
| 36  | S2    | 252 | GLN  |
| 38  | U2    | 59  | HIS  |
| 38  | U2    | 91  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | X2    | 10  | HIS  |
| 41  | X2    | 13  | HIS  |
| 42  | Y2    | 57  | GLN  |
| 44  | a2    | 33  | GLN  |
| 44  | a2    | 79  | ASN  |
| 44  | a2    | 126 | ASN  |
| 45  | b2    | 141 | GLN  |
| 45  | b2    | 181 | HIS  |
| 46  | c2    | 14  | GLN  |
| 46  | c2    | 89  | HIS  |
| 48  | f2    | 12  | HIS  |
| 48  | f2    | 14  | GLN  |
| 51  | j2    | 59  | HIS  |
| 52  | 12    | 32  | GLN  |
| 52  | 12    | 47  | GLN  |
| 52  | 12    | 169 | GLN  |
| 52  | 12    | 235 | ASN  |
| 52  | 12    | 292 | ASN  |
| 52  | 12    | 317 | GLN  |
| 53  | 62    | 31  | ASN  |
| 53  | 62    | 175 | ASN  |
| 53  | 62    | 270 | ASN  |
| 53  | 62    | 295 | GLN  |
| 53  | 62    | 296 | ASN  |
| 53  | 62    | 332 | HIS  |
| 53  | 62    | 471 | ASN  |
| 53  | 62    | 546 | GLN  |
| 54  | g2    | 55  | GLN  |
| 54  | g2    | 161 | GLN  |
| 40  | M2    | 33  | ASN  |
| 56  | A3    | 4   | ASN  |
| 56  | A3    | 11  | ASN  |
| 56  | A3    | 12  | HIS  |
| 56  | A3    | 55  | ASN  |
| 56  | A3    | 99  | ASN  |
| 56  | A3    | 170 | ASN  |
| 56  | A3    | 256 | HIS  |
| 56  | A3    | 360 | ASN  |
| 56  | A3    | 368 | HIS  |
| 56  | A3    | 413 | HIS  |
| 56  | A3    | 503 | HIS  |
| 56  | A3    | 512 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | B3    | 52  | HIS  |
| 57  | B3    | 102 | HIS  |
| 57  | B3    | 103 | GLN  |
| 57  | B3    | 195 | GLN  |
| 57  | B3    | 203 | ASN  |
| 58  | C3    | 3   | HIS  |
| 58  | C3    | 6   | HIS  |
| 58  | C3    | 12  | ASN  |
| 58  | C3    | 133 | ASN  |
| 58  | C3    | 148 | HIS  |
| 58  | C3    | 158 | HIS  |
| 58  | C3    | 204 | HIS  |
| 58  | C3    | 207 | HIS  |
| 58  | C3    | 222 | GLN  |
| 58  | C3    | 232 | HIS  |
| 59  | D3    | 32  | ASN  |
| 59  | D3    | 109 | HIS  |
| 60  | E3    | 34  | ASN  |
| 61  | F3    | 66  | ASN  |
| 62  | G3    | 51  | HIS  |
| 62  | G3    | 52  | HIS  |
| 63  | H3    | 23  | GLN  |
| 63  | H3    | 24  | ASN  |
| 63  | H3    | 25  | GLN  |
| 63  | H3    | 28  | ASN  |
| 63  | H3    | 32  | ASN  |
| 63  | H3    | 37  | HIS  |
| 65  | J3    | 3   | ASN  |
| 65  | J3    | 16  | ASN  |
| 65  | J3    | 21  | HIS  |
| 66  | K3    | 10  | HIS  |
| 66  | K3    | 15  | ASN  |
| 66  | K3    | 35  | GLN  |
| 66  | K3    | 41  | ASN  |
| 67  | L3    | 42  | HIS  |
| 68  | M3    | 39  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 74  | FMN  | 82    | 501 | -    | 33,33,33     | 1.04 | 2 (6%)      | 48,50,50    | 1.44 | 10 (20%)    |
| 69  | HEM  | O1    | 402 | 3    | 50,50,50     | 1.37 | 7 (14%)     | 67,82,82    | 1.73 | 14 (20%)    |
| 69  | HEM  | C1    | 402 | 3    | 50,50,50     | 1.27 | 6 (12%)     | 67,82,82    | 1.73 | 17 (25%)    |
| 71  | FES  | Q1    | 201 | 5    | 0,4,4        | -    | -           | -           | -    | -           |
| 72  | 3PE  | 42    | 502 | -    | 40,40,50     | 0.95 | 4 (10%)     | 43,45,55    | 1.20 | 2 (4%)      |
| 70  | HEC  | P1    | 301 | 4    | 46,50,50     | 1.89 | 7 (15%)     | 58,82,82    | 1.54 | 4 (6%)      |
| 75  | SF4  | 82    | 502 | -    | 0,12,12      | -    | -           | -           | -    | -           |
| 78  | PC1  | j2    | 201 | -    | 38,38,53     | 1.10 | 4 (10%)     | 44,46,61    | 0.99 | 2 (4%)      |
| 75  | SF4  | E2    | 302 | 23   | 0,12,12      | -    | -           | -           | -    | -           |
| 72  | 3PE  | B2    | 501 | -    | 50,50,50     | 0.89 | 4 (8%)      | 53,55,55    | 1.11 | 2 (3%)      |
| 75  | SF4  | E2    | 301 | 23   | 0,12,12      | -    | -           | -           | -    | -           |
| 75  | SF4  | A2    | 801 | 19   | 0,12,12      | -    | -           | -           | -    | -           |
| 75  | SF4  | A2    | 802 | 19   | 0,12,12      | -    | -           | -           | -    | -           |
| 70  | HEC  | D1    | 301 | 4    | 46,50,50     | 1.85 | 7 (15%)     | 58,82,82    | 1.53 | 8 (13%)     |
| 79  | HEA  | A3    | 601 | 56   | 67,67,67     | 1.21 | 4 (5%)      | 81,103,103  | 1.33 | 10 (12%)    |
| 69  | HEM  | O1    | 401 | 3    | 50,50,50     | 1.41 | 8 (16%)     | 67,82,82    | 1.88 | 18 (26%)    |
| 71  | FES  | 92    | 301 | 18   | 0,4,4        | -    | -           | -           | -    | -           |
| 75  | SF4  | D2    | 301 | -    | 0,12,12      | -    | -           | -           | -    | -           |
| 69  | HEM  | C1    | 401 | 3    | 50,50,50     | 1.31 | 7 (14%)     | 67,82,82    | 1.51 | 9 (13%)     |
| 73  | CDL  | 42    | 501 | -    | 81,81,99     | 0.97 | 7 (8%)      | 87,93,111   | 1.11 | 5 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 77  | NAP  | R2    | 601 | -    | 50,52,52     | 4.24 | 26 (52%) | 71,80,80    | 1.82 | 18 (25%) |
| 71  | FES  | A2    | 803 | 19   | 0,4,4        | -    | -        | -           | -    | -        |
| 78  | PC1  | S2    | 401 | -    | 46,46,53     | 1.00 | 4 (8%)   | 52,54,61    | 1.05 | 2 (3%)   |
| 72  | 3PE  | 22    | 401 | -    | 40,40,50     | 0.95 | 3 (7%)   | 43,45,55    | 1.14 | 2 (4%)   |
| 79  | HEA  | A3    | 602 | 56   | 67,67,67     | 1.19 | 7 (10%)  | 81,103,103  | 1.35 | 13 (16%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 74  | FMN  | 82    | 501 | -    | -       | 8/18/18/18   | 0/3/3/3 |
| 69  | HEM  | O1    | 402 | 3    | -       | 4/14/54/54   | -       |
| 69  | HEM  | C1    | 402 | 3    | -       | 6/14/54/54   | -       |
| 71  | FES  | Q1    | 201 | 5    | -       | -            | 0/1/1/1 |
| 72  | 3PE  | 42    | 502 | -    | -       | 25/44/44/54  | -       |
| 70  | HEC  | P1    | 301 | 4    | -       | 10/14/54/54  | -       |
| 75  | SF4  | 82    | 502 | -    | -       | -            | 0/6/5/5 |
| 78  | PC1  | j2    | 201 | -    | -       | 19/42/42/57  | -       |
| 75  | SF4  | E2    | 302 | 23   | -       | -            | 0/6/5/5 |
| 72  | 3PE  | B2    | 501 | -    | -       | 26/54/54/54  | -       |
| 75  | SF4  | E2    | 301 | 23   | -       | -            | 0/6/5/5 |
| 75  | SF4  | A2    | 801 | 19   | -       | -            | 0/6/5/5 |
| 75  | SF4  | A2    | 802 | 19   | -       | -            | 0/6/5/5 |
| 79  | HEA  | A3    | 601 | 56   | -       | 7/36/76/76   | -       |
| 70  | HEC  | D1    | 301 | 4    | -       | 8/14/54/54   | -       |
| 69  | HEM  | O1    | 401 | 3    | -       | 6/14/54/54   | -       |
| 71  | FES  | 92    | 301 | 18   | -       | -            | 0/1/1/1 |
| 75  | SF4  | D2    | 301 | -    | -       | -            | 0/6/5/5 |
| 69  | HEM  | C1    | 401 | 3    | -       | 4/14/54/54   | -       |
| 73  | CDL  | 42    | 501 | -    | -       | 41/92/92/110 | -       |
| 77  | NAP  | R2    | 601 | -    | -       | 17/35/67/67  | 0/5/5/5 |
| 71  | FES  | A2    | 803 | 19   | -       | -            | 0/1/1/1 |
| 78  | PC1  | S2    | 401 | -    | -       | 20/50/50/57  | -       |
| 72  | 3PE  | 22    | 401 | -    | -       | 20/44/44/54  | -       |
| 79  | HEA  | A3    | 602 | 56   | -       | 7/36/76/76   | -       |

All (107) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 77  | R2    | 601 | NAP  | O4D-C1D | 17.22 | 1.63        | 1.40     |
| 77  | R2    | 601 | NAP  | C2B-C1B | -9.50 | 1.29        | 1.53     |
| 77  | R2    | 601 | NAP  | PN-O3   | 8.68  | 1.68        | 1.59     |
| 77  | R2    | 601 | NAP  | O4B-C1B | 8.64  | 1.62        | 1.42     |
| 77  | R2    | 601 | NAP  | C7N-N7N | 7.50  | 1.46        | 1.33     |
| 70  | P1    | 301 | HEC  | CAB-C3B | 6.65  | 1.56        | 1.35     |
| 77  | R2    | 601 | NAP  | O4D-C4D | -6.63 | 1.30        | 1.45     |
| 70  | P1    | 301 | HEC  | CAC-C3C | 6.46  | 1.56        | 1.35     |
| 70  | D1    | 301 | HEC  | CAB-C3B | 6.46  | 1.56        | 1.35     |
| 70  | D1    | 301 | HEC  | CAC-C3C | 6.33  | 1.55        | 1.35     |
| 77  | R2    | 601 | NAP  | O4B-C4B | -5.78 | 1.32        | 1.45     |
| 77  | R2    | 601 | NAP  | PA-O3   | 5.76  | 1.65        | 1.59     |
| 77  | R2    | 601 | NAP  | C3N-C7N | 5.41  | 1.58        | 1.50     |
| 77  | R2    | 601 | NAP  | C5A-N7A | -4.42 | 1.31        | 1.39     |
| 77  | R2    | 601 | NAP  | C6A-N6A | 4.20  | 1.44        | 1.34     |
| 79  | A3    | 601 | HEA  | C11-C3B | -4.09 | 1.46        | 1.51     |
| 77  | R2    | 601 | NAP  | O3D-C3D | -3.99 | 1.33        | 1.43     |
| 70  | D1    | 301 | HEC  | CBB-CAB | -3.72 | 1.35        | 1.49     |
| 70  | P1    | 301 | HEC  | CBC-CAC | -3.68 | 1.35        | 1.49     |
| 79  | A3    | 602 | HEA  | CMA-C3A | -3.62 | 1.37        | 1.45     |
| 70  | D1    | 301 | HEC  | CBC-CAC | -3.54 | 1.36        | 1.49     |
| 70  | P1    | 301 | HEC  | CBB-CAB | -3.48 | 1.36        | 1.49     |
| 77  | R2    | 601 | NAP  | O7N-C7N | -3.46 | 1.17        | 1.24     |
| 69  | C1    | 401 | HEM  | CAB-C3B | 3.46  | 1.56        | 1.47     |
| 69  | O1    | 402 | HEM  | FE-NA   | 3.43  | 2.06        | 1.95     |
| 69  | O1    | 401 | HEM  | CAB-C3B | 3.38  | 1.56        | 1.47     |
| 69  | O1    | 402 | HEM  | FE-NC   | 3.36  | 2.06        | 1.95     |
| 77  | R2    | 601 | NAP  | O2D-C2D | 3.35  | 1.51        | 1.43     |
| 69  | C1    | 401 | HEM  | FE-NB   | 3.16  | 2.04        | 1.94     |
| 69  | C1    | 402 | HEM  | CHB-C4A | -3.09 | 1.32        | 1.39     |
| 69  | O1    | 401 | HEM  | FE-NB   | 3.09  | 2.04        | 1.94     |
| 69  | C1    | 401 | HEM  | C3B-C2B | -3.02 | 1.31        | 1.37     |
| 79  | A3    | 602 | HEA  | FE-NA   | 2.95  | 2.04        | 1.95     |
| 74  | 82    | 501 | FMN  | C4A-N5  | 2.93  | 1.37        | 1.30     |
| 72  | B2    | 501 | 3PE  | O21-C2  | -2.90 | 1.39        | 1.46     |
| 77  | R2    | 601 | NAP  | C4A-N9A | -2.82 | 1.31        | 1.37     |
| 73  | 42    | 501 | CDL  | OA6-CA4 | -2.82 | 1.40        | 1.46     |
| 78  | j2    | 201 | PC1  | O21-C2  | -2.74 | 1.40        | 1.46     |
| 79  | A3    | 601 | HEA  | C1A-C2A | -2.74 | 1.40        | 1.45     |
| 69  | O1    | 401 | HEM  | C1B-C2B | 2.72  | 1.50        | 1.44     |
| 77  | R2    | 601 | NAP  | PA-O5B  | 2.71  | 1.70        | 1.59     |
| 69  | O1    | 402 | HEM  | CAC-C3C | 2.71  | 1.54        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 78  | S2    | 401 | PC1  | O21-C2  | -2.66 | 1.40        | 1.46     |
| 77  | R2    | 601 | NAP  | P2B-O2B | 2.63  | 1.64        | 1.59     |
| 79  | A3    | 601 | HEA  | CMA-C3A | -2.62 | 1.39        | 1.45     |
| 77  | R2    | 601 | NAP  | C8A-N9A | -2.62 | 1.33        | 1.37     |
| 77  | R2    | 601 | NAP  | O3B-C3B | -2.61 | 1.36        | 1.43     |
| 69  | O1    | 401 | HEM  | CAC-C3C | 2.60  | 1.54        | 1.47     |
| 73  | 42    | 501 | CDL  | OB6-CB5 | 2.58  | 1.41        | 1.34     |
| 79  | A3    | 602 | HEA  | C1D-C2D | 2.58  | 1.49        | 1.44     |
| 79  | A3    | 602 | HEA  | C1D-ND  | -2.57 | 1.35        | 1.40     |
| 69  | O1    | 402 | HEM  | C1A-NA  | 2.49  | 1.44        | 1.39     |
| 69  | C1    | 401 | HEM  | FE-ND   | 2.48  | 2.02        | 1.94     |
| 72  | 42    | 502 | 3PE  | O21-C21 | 2.46  | 1.41        | 1.34     |
| 77  | R2    | 601 | NAP  | C4N-C3N | -2.45 | 1.35        | 1.39     |
| 72  | 22    | 401 | 3PE  | O21-C21 | 2.44  | 1.41        | 1.34     |
| 73  | 42    | 501 | CDL  | OA8-CA7 | 2.44  | 1.40        | 1.33     |
| 79  | A3    | 602 | HEA  | C3A-C2A | -2.44 | 1.31        | 1.37     |
| 72  | 22    | 401 | 3PE  | O31-C31 | 2.44  | 1.40        | 1.33     |
| 69  | C1    | 401 | HEM  | CAC-C3C | 2.43  | 1.53        | 1.47     |
| 78  | S2    | 401 | PC1  | O31-C31 | 2.42  | 1.40        | 1.33     |
| 77  | R2    | 601 | NAP  | C5A-C4A | -2.40 | 1.34        | 1.39     |
| 69  | O1    | 402 | HEM  | FE-NB   | 2.39  | 2.02        | 1.94     |
| 79  | A3    | 602 | HEA  | CMD-C2D | 2.37  | 1.55        | 1.50     |
| 70  | P1    | 301 | HEC  | C3C-C2C | -2.36 | 1.33        | 1.41     |
| 73  | 42    | 501 | CDL  | OB8-CB7 | 2.36  | 1.40        | 1.33     |
| 72  | B2    | 501 | 3PE  | O31-C3  | -2.34 | 1.39        | 1.45     |
| 72  | 42    | 502 | 3PE  | O31-C3  | -2.33 | 1.40        | 1.45     |
| 79  | A3    | 601 | HEA  | C3A-C4A | -2.33 | 1.42        | 1.46     |
| 77  | R2    | 601 | NAP  | PN-O5D  | 2.31  | 1.68        | 1.59     |
| 69  | O1    | 401 | HEM  | C2A-C3A | -2.30 | 1.32        | 1.38     |
| 69  | C1    | 402 | HEM  | FE-ND   | 2.29  | 2.02        | 1.94     |
| 69  | O1    | 401 | HEM  | C3D-C2D | -2.29 | 1.31        | 1.36     |
| 70  | D1    | 301 | HEC  | C3B-C2B | -2.29 | 1.33        | 1.41     |
| 73  | 42    | 501 | CDL  | OB8-CB6 | -2.28 | 1.40        | 1.45     |
| 69  | C1    | 402 | HEM  | FE-NC   | 2.27  | 2.02        | 1.95     |
| 72  | B2    | 501 | 3PE  | O31-C31 | 2.27  | 1.40        | 1.33     |
| 72  | B2    | 501 | 3PE  | O21-C21 | 2.27  | 1.40        | 1.34     |
| 69  | O1    | 402 | HEM  | CAB-C3B | 2.26  | 1.53        | 1.47     |
| 72  | 42    | 502 | 3PE  | O31-C31 | 2.26  | 1.39        | 1.33     |
| 78  | j2    | 201 | PC1  | O31-C31 | 2.25  | 1.39        | 1.33     |
| 69  | C1    | 401 | HEM  | C2A-C3A | -2.24 | 1.33        | 1.38     |
| 74  | 82    | 501 | FMN  | C10-N1  | 2.24  | 1.37        | 1.33     |
| 70  | P1    | 301 | HEC  | C3B-C2B | -2.24 | 1.33        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 78  | j2    | 201 | PC1  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 69  | O1    | 402 | HEM  | C2A-C3A | -2.20 | 1.33        | 1.38     |
| 77  | R2    | 601 | NAP  | C5N-C4N | -2.20 | 1.35        | 1.38     |
| 70  | D1    | 301 | HEC  | C3C-C2C | -2.16 | 1.33        | 1.41     |
| 69  | C1    | 402 | HEM  | FE-NB   | 2.16  | 2.01        | 1.94     |
| 77  | R2    | 601 | NAP  | O2B-C2B | 2.16  | 1.51        | 1.44     |
| 69  | O1    | 401 | HEM  | FE-NA   | 2.15  | 2.02        | 1.95     |
| 69  | C1    | 402 | HEM  | CAB-C3B | 2.14  | 1.53        | 1.47     |
| 70  | P1    | 301 | HEC  | C3D-C2D | -2.10 | 1.33        | 1.38     |
| 78  | j2    | 201 | PC1  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 78  | S2    | 401 | PC1  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 79  | A3    | 602 | HEA  | FE-NC   | 2.09  | 2.02        | 1.95     |
| 73  | 42    | 501 | CDL  | OB6-CB4 | -2.07 | 1.41        | 1.46     |
| 69  | C1    | 401 | HEM  | CMB-C2B | 2.07  | 1.55        | 1.50     |
| 73  | 42    | 501 | CDL  | OA8-CA6 | -2.06 | 1.40        | 1.45     |
| 78  | S2    | 401 | PC1  | O31-C3  | -2.06 | 1.40        | 1.45     |
| 69  | O1    | 401 | HEM  | CMD-C2D | 2.06  | 1.55        | 1.50     |
| 72  | 22    | 401 | 3PE  | O31-C3  | -2.05 | 1.40        | 1.45     |
| 77  | R2    | 601 | NAP  | C5B-C4B | 2.04  | 1.57        | 1.51     |
| 77  | R2    | 601 | NAP  | C5D-C4D | 2.04  | 1.57        | 1.51     |
| 69  | C1    | 402 | HEM  | C1C-C2C | 2.02  | 1.49        | 1.45     |
| 72  | 42    | 502 | 3PE  | O21-C2  | -2.01 | 1.41        | 1.46     |
| 70  | D1    | 301 | HEC  | CMD-C2D | 2.01  | 1.54        | 1.50     |

All (136) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 70  | D1    | 301 | HEC  | CBC-CAC-C3C | -6.72 | 113.99      | 127.43   |
| 70  | P1    | 301 | HEC  | CBB-CAB-C3B | -6.68 | 114.09      | 127.43   |
| 70  | P1    | 301 | HEC  | CBC-CAC-C3C | -6.08 | 115.28      | 127.43   |
| 77  | R2    | 601 | NAP  | N3A-C2A-N1A | -5.93 | 119.60      | 128.58   |
| 69  | O1    | 401 | HEM  | C3B-C2B-C1B | -5.35 | 102.40      | 106.41   |
| 69  | O1    | 402 | HEM  | C3B-C2B-C1B | 4.98  | 110.15      | 106.41   |
| 70  | D1    | 301 | HEC  | CBB-CAB-C3B | -4.98 | 117.48      | 127.43   |
| 69  | O1    | 401 | HEM  | CMA-C3A-C4A | -4.94 | 117.90      | 125.42   |
| 69  | C1    | 401 | HEM  | CBD-CAD-C3D | 4.79  | 125.78      | 112.53   |
| 77  | R2    | 601 | NAP  | N6A-C6A-N1A | -4.74 | 107.81      | 118.38   |
| 77  | R2    | 601 | NAP  | C5A-C4A-N3A | -4.69 | 120.26      | 126.72   |
| 72  | 22    | 401 | 3PE  | O21-C21-C22 | 4.34  | 120.88      | 111.48   |
| 77  | R2    | 601 | NAP  | N9A-C8A-N7A | -4.29 | 107.85      | 113.94   |
| 72  | 42    | 502 | 3PE  | O21-C21-C22 | 4.23  | 120.63      | 111.48   |
| 69  | O1    | 402 | HEM  | C2A-C1A-NA  | -4.21 | 105.48      | 110.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 78  | S2    | 401 | PC1  | O21-C21-C22 | 4.17  | 120.51      | 111.48   |
| 73  | 42    | 501 | CDL  | OA6-CA5-C11 | 4.17  | 120.50      | 111.48   |
| 79  | A3    | 601 | HEA  | C17-C18-C19 | -4.16 | 118.10      | 127.62   |
| 69  | O1    | 402 | HEM  | CHC-C4B-NB  | 4.12  | 128.86      | 124.42   |
| 69  | C1    | 401 | HEM  | O1D-CGD-CBD | -4.05 | 110.25      | 123.09   |
| 72  | B2    | 501 | 3PE  | O21-C21-C22 | 3.92  | 119.95      | 111.48   |
| 69  | O1    | 402 | HEM  | CHA-C1A-C2A | 3.90  | 133.83      | 125.30   |
| 69  | C1    | 401 | HEM  | CBB-CAB-C3B | -3.87 | 108.20      | 127.53   |
| 69  | C1    | 402 | HEM  | CAA-CBA-CGA | 3.81  | 123.78      | 113.67   |
| 69  | O1    | 402 | HEM  | CHB-C1B-NB  | -3.77 | 119.71      | 124.37   |
| 73  | 42    | 501 | CDL  | OB6-CB5-C51 | 3.74  | 119.58      | 111.48   |
| 69  | O1    | 401 | HEM  | C2B-C1B-NB  | 3.72  | 114.12      | 109.84   |
| 74  | 82    | 501 | FMN  | C4-N3-C2    | -3.72 | 119.04      | 125.64   |
| 77  | R2    | 601 | NAP  | C4D-O4D-C1D | -3.63 | 106.61      | 109.92   |
| 69  | O1    | 401 | HEM  | O1D-CGD-CBD | -3.62 | 111.60      | 123.09   |
| 69  | O1    | 401 | HEM  | C4B-C3B-C2B | 3.58  | 110.57      | 107.28   |
| 69  | O1    | 401 | HEM  | CHB-C1B-NB  | -3.49 | 120.04      | 124.37   |
| 69  | C1    | 402 | HEM  | C3C-C2C-C1C | -3.46 | 103.77      | 107.05   |
| 77  | R2    | 601 | NAP  | C5A-C6A-N6A | 3.46  | 131.86      | 123.29   |
| 69  | C1    | 402 | HEM  | CMA-C3A-C4A | -3.46 | 120.16      | 125.42   |
| 69  | O1    | 401 | HEM  | O2D-CGD-O1D | 3.44  | 132.19      | 123.33   |
| 77  | R2    | 601 | NAP  | C2A-N3A-C4A | 3.40  | 120.12      | 111.83   |
| 69  | C1    | 402 | HEM  | CHD-C1D-ND  | 3.37  | 128.05      | 124.42   |
| 79  | A3    | 601 | HEA  | C13-C14-C15 | -3.33 | 120.00      | 127.62   |
| 69  | O1    | 401 | HEM  | CMA-C3A-C2A | 3.31  | 132.64      | 125.62   |
| 79  | A3    | 602 | HEA  | CHA-C1A-NA  | -3.25 | 120.91      | 124.45   |
| 69  | C1    | 402 | HEM  | C4D-ND-C1D  | 3.11  | 108.89      | 105.21   |
| 74  | 82    | 501 | FMN  | O4-C4-C4A   | -3.10 | 118.35      | 126.53   |
| 69  | O1    | 402 | HEM  | O1D-CGD-CBD | -3.08 | 113.31      | 123.09   |
| 69  | C1    | 402 | HEM  | O2A-CGA-CBA | 3.07  | 123.70      | 114.00   |
| 69  | C1    | 402 | HEM  | C4A-CHB-C1B | 2.97  | 133.23      | 126.25   |
| 79  | A3    | 601 | HEA  | C1B-C2B-C3B | 2.93  | 110.18      | 106.80   |
| 69  | C1    | 402 | HEM  | CHC-C1C-NC  | -2.88 | 121.32      | 124.45   |
| 74  | 82    | 501 | FMN  | C4A-C4-N3   | 2.86  | 120.54      | 113.25   |
| 77  | R2    | 601 | NAP  | C5A-N7A-C8A | 2.85  | 107.93      | 103.45   |
| 69  | C1    | 402 | HEM  | CMA-C3A-C2A | 2.83  | 131.63      | 125.62   |
| 74  | 82    | 501 | FMN  | C5A-C9A-N10 | 2.83  | 120.53      | 117.97   |
| 69  | C1    | 402 | HEM  | O2A-CGA-O1A | -2.83 | 116.06      | 123.33   |
| 69  | C1    | 401 | HEM  | O2A-CGA-O1A | 2.81  | 130.56      | 123.33   |
| 69  | C1    | 402 | HEM  | CHB-C1B-NB  | -2.80 | 120.90      | 124.37   |
| 74  | 82    | 501 | FMN  | C4A-C10-N1  | -2.77 | 117.79      | 124.59   |
| 74  | 82    | 501 | FMN  | C5'-C4'-C3' | -2.75 | 107.02      | 112.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69  | O1    | 402 | HEM  | CAA-C2A-C1A | -2.75 | 119.57      | 124.94   |
| 69  | O1    | 401 | HEM  | CMD-C2D-C1D | -2.73 | 120.77      | 125.03   |
| 69  | C1    | 401 | HEM  | CMB-C2B-C1B | -2.73 | 120.77      | 125.03   |
| 73  | 42    | 501 | CDL  | OA8-CA7-C31 | 2.69  | 120.02      | 111.83   |
| 70  | P1    | 301 | HEC  | O1D-CGD-CBD | -2.68 | 114.58      | 123.09   |
| 73  | 42    | 501 | CDL  | OB8-CB7-C71 | 2.67  | 119.99      | 111.83   |
| 69  | C1    | 402 | HEM  | CAD-CBD-CGD | 2.66  | 120.72      | 113.67   |
| 72  | B2    | 501 | 3PE  | O31-C31-C32 | 2.65  | 119.92      | 111.83   |
| 72  | 22    | 401 | 3PE  | O31-C31-C32 | 2.63  | 119.84      | 111.83   |
| 69  | C1    | 402 | HEM  | CBD-CAD-C3D | 2.62  | 119.77      | 112.53   |
| 77  | R2    | 601 | NAP  | C4A-N9A-C1B | -2.62 | 120.51      | 126.63   |
| 78  | S2    | 401 | PC1  | O31-C31-C32 | 2.61  | 119.81      | 111.83   |
| 69  | O1    | 401 | HEM  | C1B-NB-C4B  | -2.59 | 102.14      | 105.21   |
| 69  | O1    | 401 | HEM  | CAB-C3B-C2B | -2.59 | 120.02      | 128.43   |
| 78  | j2    | 201 | PC1  | O21-C21-C22 | 2.58  | 120.41      | 110.93   |
| 78  | j2    | 201 | PC1  | O31-C31-C32 | 2.57  | 119.68      | 111.83   |
| 70  | D1    | 301 | HEC  | O1A-CGA-CBA | -2.56 | 114.97      | 123.09   |
| 79  | A3    | 602 | HEA  | CMD-C2D-C1D | 2.54  | 129.00      | 125.03   |
| 69  | C1    | 402 | HEM  | CAA-C2A-C1A | -2.51 | 120.03      | 124.94   |
| 69  | O1    | 401 | HEM  | CBD-CAD-C3D | 2.51  | 119.47      | 112.53   |
| 69  | C1    | 401 | HEM  | O2D-CGD-CBD | 2.51  | 121.92      | 114.00   |
| 72  | 42    | 502 | 3PE  | O31-C31-C32 | 2.50  | 119.47      | 111.83   |
| 77  | R2    | 601 | NAP  | N3A-C4A-N9A | 2.48  | 131.39      | 127.17   |
| 79  | A3    | 602 | HEA  | C1D-C2D-C3D | -2.47 | 104.39      | 106.98   |
| 69  | O1    | 402 | HEM  | CMB-C2B-C3B | -2.46 | 122.47      | 128.43   |
| 79  | A3    | 601 | HEA  | C17-C16-C15 | -2.46 | 105.05      | 113.19   |
| 79  | A3    | 602 | HEA  | C12-C11-C3B | 2.44  | 115.94      | 112.12   |
| 77  | R2    | 601 | NAP  | C6N-N1N-C2N | -2.44 | 119.80      | 121.88   |
| 79  | A3    | 602 | HEA  | C4A-C3A-C2A | 2.43  | 108.92      | 106.81   |
| 69  | O1    | 401 | HEM  | CHA-C4D-ND  | -2.43 | 121.37      | 124.37   |
| 69  | O1    | 401 | HEM  | CMB-C2B-C3B | 2.42  | 134.29      | 128.43   |
| 70  | D1    | 301 | HEC  | O2D-CGD-O1D | 2.42  | 129.55      | 123.33   |
| 79  | A3    | 602 | HEA  | C13-C14-C15 | -2.42 | 122.10      | 127.62   |
| 69  | C1    | 401 | HEM  | CMA-C3A-C4A | -2.41 | 121.74      | 125.42   |
| 69  | C1    | 402 | HEM  | C4C-NC-C1C  | -2.39 | 101.92      | 105.82   |
| 69  | C1    | 402 | HEM  | C3D-C4D-ND  | -2.36 | 107.58      | 110.17   |
| 79  | A3    | 601 | HEA  | C3C-C4C-NC  | 2.35  | 111.78      | 109.80   |
| 79  | A3    | 601 | HEA  | CAD-C3D-C4D | 2.33  | 128.76      | 124.70   |
| 77  | R2    | 601 | NAP  | C5A-C4A-N9A | 2.32  | 108.34      | 105.81   |
| 69  | O1    | 402 | HEM  | C4B-C3B-C2B | -2.31 | 105.15      | 107.28   |
| 70  | D1    | 301 | HEC  | O1D-CGD-CBD | -2.30 | 115.81      | 123.09   |
| 77  | R2    | 601 | NAP  | C4A-C5A-N7A | -2.29 | 107.97      | 110.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 70  | D1    | 301 | HEC  | CAD-C3D-C2D | 2.26  | 132.14      | 127.07   |
| 79  | A3    | 602 | HEA  | CMB-C2B-C3B | -2.26 | 125.91      | 130.28   |
| 69  | O1    | 402 | HEM  | O2D-CGD-CBD | 2.26  | 121.13      | 114.00   |
| 79  | A3    | 602 | HEA  | C25-C23-C24 | 2.26  | 119.78      | 114.59   |
| 74  | 82    | 501 | FMN  | C10-N1-C2   | 2.25  | 121.73      | 116.85   |
| 69  | O1    | 401 | HEM  | C4A-C3A-C2A | 2.25  | 109.40      | 106.82   |
| 79  | A3    | 602 | HEA  | CAA-C2A-C1A | 2.23  | 129.39      | 124.85   |
| 69  | C1    | 402 | HEM  | C2A-C1A-NA  | -2.23 | 107.68      | 110.15   |
| 74  | 82    | 501 | FMN  | C4-C4A-C10  | 2.23  | 120.75      | 116.93   |
| 69  | C1    | 401 | HEM  | CHC-C1C-NC  | 2.20  | 126.85      | 124.45   |
| 79  | A3    | 601 | HEA  | C4B-C3B-C2B | -2.19 | 103.75      | 107.44   |
| 74  | 82    | 501 | FMN  | C4A-C10-N10 | 2.19  | 119.61      | 116.48   |
| 69  | O1    | 401 | HEM  | C3C-C2C-C1C | 2.17  | 109.09      | 107.05   |
| 79  | A3    | 602 | HEA  | C26-C15-C16 | 2.17  | 118.99      | 115.23   |
| 69  | O1    | 402 | HEM  | CMD-C2D-C1D | -2.17 | 121.65      | 125.03   |
| 74  | 82    | 501 | FMN  | C9A-C5A-N5  | -2.17 | 120.16      | 122.45   |
| 79  | A3    | 601 | HEA  | C12-C13-C14 | -2.15 | 106.51      | 112.16   |
| 69  | O1    | 402 | HEM  | CHA-C1A-NA  | -2.14 | 119.98      | 123.86   |
| 77  | R2    | 601 | NAP  | C3N-C7N-N7N | 2.14  | 120.38      | 117.74   |
| 69  | O1    | 402 | HEM  | CMC-C2C-C1C | -2.12 | 120.99      | 124.73   |
| 79  | A3    | 601 | HEA  | C20-C19-C18 | 2.11  | 125.91      | 121.17   |
| 79  | A3    | 602 | HEA  | CBD-CAD-C3D | 2.10  | 118.34      | 112.53   |
| 77  | R2    | 601 | NAP  | C4B-O4B-C1B | -2.09 | 104.85      | 109.47   |
| 69  | O1    | 401 | HEM  | O1A-CGA-CBA | -2.09 | 116.48      | 123.09   |
| 73  | 42    | 501 | CDL  | CA4-OA6-CA5 | -2.08 | 112.82      | 117.80   |
| 70  | D1    | 301 | HEC  | CAD-C3D-C4D | -2.08 | 120.89      | 124.94   |
| 69  | O1    | 402 | HEM  | CHC-C4B-C3B | -2.07 | 120.95      | 125.07   |
| 77  | R2    | 601 | NAP  | C4A-N9A-C8A | 2.06  | 107.91      | 105.74   |
| 79  | A3    | 602 | HEA  | C3C-C4C-NC  | 2.06  | 111.53      | 109.80   |
| 69  | C1    | 401 | HEM  | CMA-C3A-C2A | 2.05  | 129.96      | 125.62   |
| 69  | O1    | 401 | HEM  | CHA-C4D-C3D | 2.04  | 128.99      | 125.23   |
| 79  | A3    | 601 | HEA  | C27-C19-C18 | -2.04 | 118.40      | 123.63   |
| 70  | P1    | 301 | HEC  | O1A-CGA-CBA | -2.03 | 116.64      | 123.09   |
| 77  | R2    | 601 | NAP  | C1B-N9A-C8A | 2.02  | 131.58      | 127.09   |
| 77  | R2    | 601 | NAP  | C2B-C1B-N9A | -2.01 | 110.44      | 113.75   |
| 70  | D1    | 301 | HEC  | CMD-C2D-C1D | -2.00 | 122.37      | 125.42   |
| 79  | A3    | 602 | HEA  | C3A-C2A-C1A | -2.00 | 105.15      | 107.05   |

There are no chirality outliers.

All (228) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 69  | O1    | 401 | HEM  | C2B-C3B-CAB-CBB |
| 70  | D1    | 301 | HEC  | C2B-C3B-CAB-CBB |
| 70  | D1    | 301 | HEC  | C4B-C3B-CAB-CBB |
| 70  | D1    | 301 | HEC  | C2C-C3C-CAC-CBC |
| 70  | D1    | 301 | HEC  | C4C-C3C-CAC-CBC |
| 70  | P1    | 301 | HEC  | C2B-C3B-CAB-CBB |
| 70  | P1    | 301 | HEC  | C2C-C3C-CAC-CBC |
| 70  | P1    | 301 | HEC  | C4C-C3C-CAC-CBC |
| 72  | 22    | 401 | 3PE  | C1-O11-P-O14    |
| 72  | 22    | 401 | 3PE  | C22-C21-O21-C2  |
| 72  | 42    | 502 | 3PE  | C11-O13-P-O11   |
| 72  | 42    | 502 | 3PE  | C11-O13-P-O12   |
| 72  | 42    | 502 | 3PE  | C11-O13-P-O14   |
| 72  | 42    | 502 | 3PE  | C2-C1-O11-P     |
| 72  | 42    | 502 | 3PE  | O13-C11-C12-N   |
| 72  | 42    | 502 | 3PE  | C22-C21-O21-C2  |
| 72  | B2    | 501 | 3PE  | C1-O11-P-O13    |
| 72  | B2    | 501 | 3PE  | O11-C1-C2-O21   |
| 72  | B2    | 501 | 3PE  | O22-C21-O21-C2  |
| 72  | B2    | 501 | 3PE  | C22-C21-O21-C2  |
| 73  | 42    | 501 | CDL  | CA2-OA2-PA1-OA4 |
| 73  | 42    | 501 | CDL  | CA2-OA2-PA1-OA5 |
| 73  | 42    | 501 | CDL  | OA6-CA4-CA6-OA8 |
| 73  | 42    | 501 | CDL  | OA7-CA5-OA6-CA4 |
| 73  | 42    | 501 | CDL  | C11-CA5-OA6-CA4 |
| 73  | 42    | 501 | CDL  | CB2-OB2-PB2-OB4 |
| 73  | 42    | 501 | CDL  | CB2-OB2-PB2-OB5 |
| 74  | 82    | 501 | FMN  | N10-C1'-C2'-O2' |
| 74  | 82    | 501 | FMN  | N10-C1'-C2'-C3' |
| 74  | 82    | 501 | FMN  | C5'-O5'-P-O2P   |
| 74  | 82    | 501 | FMN  | C5'-O5'-P-O3P   |
| 77  | R2    | 601 | NAP  | C5B-O5B-PA-O1A  |
| 77  | R2    | 601 | NAP  | C5B-O5B-PA-O2A  |
| 77  | R2    | 601 | NAP  | C5B-O5B-PA-O3   |
| 77  | R2    | 601 | NAP  | C1B-C2B-O2B-P2B |
| 77  | R2    | 601 | NAP  | PA-O3-PN-O5D    |
| 77  | R2    | 601 | NAP  | C5D-O5D-PN-O3   |
| 77  | R2    | 601 | NAP  | C5D-O5D-PN-O2N  |
| 77  | R2    | 601 | NAP  | C2D-C1D-N1N-C2N |
| 77  | R2    | 601 | NAP  | C2D-C1D-N1N-C6N |
| 78  | S2    | 401 | PC1  | C11-O13-P-O12   |
| 78  | S2    | 401 | PC1  | C11-O13-P-O11   |
| 78  | j2    | 201 | PC1  | C11-O13-P-O12   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 78  | j2    | 201 | PC1  | C11-O13-P-O14   |
| 78  | j2    | 201 | PC1  | C11-O13-P-O11   |
| 78  | j2    | 201 | PC1  | O22-C21-O21-C2  |
| 79  | A3    | 601 | HEA  | C2A-C3A-CMA-OMA |
| 79  | A3    | 601 | HEA  | C4A-C3A-CMA-OMA |
| 79  | A3    | 602 | HEA  | C2A-C3A-CMA-OMA |
| 79  | A3    | 602 | HEA  | C4A-C3A-CMA-OMA |
| 72  | 42    | 502 | 3PE  | O32-C31-O31-C3  |
| 72  | 22    | 401 | 3PE  | O22-C21-O21-C2  |
| 72  | 42    | 502 | 3PE  | O22-C21-O21-C2  |
| 72  | 42    | 502 | 3PE  | C32-C31-O31-C3  |
| 78  | j2    | 201 | PC1  | C22-C21-O21-C2  |
| 73  | 42    | 501 | CDL  | C71-CB7-OB8-CB6 |
| 73  | 42    | 501 | CDL  | OB9-CB7-OB8-CB6 |
| 78  | S2    | 401 | PC1  | O22-C21-O21-C2  |
| 78  | S2    | 401 | PC1  | C22-C21-O21-C2  |
| 79  | A3    | 601 | HEA  | C15-C16-C17-C18 |
| 73  | 42    | 501 | CDL  | C31-CA7-OA8-CA6 |
| 77  | R2    | 601 | NAP  | O4B-C4B-C5B-O5B |
| 77  | R2    | 601 | NAP  | O4D-C4D-C5D-O5D |
| 73  | 42    | 501 | CDL  | CB5-C51-C52-C53 |
| 72  | B2    | 501 | 3PE  | C21-C22-C23-C24 |
| 73  | 42    | 501 | CDL  | CA5-C11-C12-C13 |
| 73  | 42    | 501 | CDL  | OA9-CA7-OA8-CA6 |
| 73  | 42    | 501 | CDL  | C51-CB5-OB6-CB4 |
| 73  | 42    | 501 | CDL  | OB7-CB5-OB6-CB4 |
| 73  | 42    | 501 | CDL  | C1-CA2-OA2-PA1  |
| 72  | 22    | 401 | 3PE  | C21-C22-C23-C24 |
| 73  | 42    | 501 | CDL  | C13-C14-C15-C16 |
| 72  | 22    | 401 | 3PE  | C2C-C2D-C2E-C2F |
| 73  | 42    | 501 | CDL  | C78-C79-C80-C81 |
| 73  | 42    | 501 | CDL  | CA7-C31-C32-C33 |
| 72  | B2    | 501 | 3PE  | C23-C24-C25-C26 |
| 73  | 42    | 501 | CDL  | C73-C74-C75-C76 |
| 72  | 22    | 401 | 3PE  | C32-C31-O31-C3  |
| 78  | S2    | 401 | PC1  | C25-C26-C27-C28 |
| 73  | 42    | 501 | CDL  | C72-C73-C74-C75 |
| 78  | S2    | 401 | PC1  | C33-C34-C35-C36 |
| 72  | 22    | 401 | 3PE  | C32-C33-C34-C35 |
| 73  | 42    | 501 | CDL  | C77-C78-C79-C80 |
| 73  | 42    | 501 | CDL  | C74-C75-C76-C77 |
| 72  | 42    | 502 | 3PE  | C28-C29-C2A-C2B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 72  | B2    | 501 | 3PE  | C37-C38-C39-C3A |
| 72  | 22    | 401 | 3PE  | O32-C31-O31-C3  |
| 69  | O1    | 401 | HEM  | C4B-C3B-CAB-CBB |
| 72  | B2    | 501 | 3PE  | C2E-C2F-C2G-C2H |
| 72  | B2    | 501 | 3PE  | C31-C32-C33-C34 |
| 78  | S2    | 401 | PC1  | O11-C1-C2-C3    |
| 73  | 42    | 501 | CDL  | C75-C76-C77-C78 |
| 72  | 42    | 502 | 3PE  | C34-C35-C36-C37 |
| 72  | 42    | 502 | 3PE  | C23-C24-C25-C26 |
| 70  | P1    | 301 | HEC  | C1A-C2A-CAA-CBA |
| 72  | 22    | 401 | 3PE  | C1-C2-C3-O31    |
| 78  | j2    | 201 | PC1  | C1-C2-C3-O31    |
| 72  | B2    | 501 | 3PE  | C35-C36-C37-C38 |
| 73  | 42    | 501 | CDL  | C80-C81-C82-C83 |
| 74  | 82    | 501 | FMN  | C5'-O5'-P-O1P   |
| 72  | 22    | 401 | 3PE  | C3-C2-O21-C21   |
| 73  | 42    | 501 | CDL  | C83-C84-C85-C86 |
| 73  | 42    | 501 | CDL  | OA5-CA3-CA4-OA6 |
| 78  | j2    | 201 | PC1  | C32-C31-O31-C3  |
| 72  | 22    | 401 | 3PE  | C28-C29-C2A-C2B |
| 72  | B2    | 501 | 3PE  | C27-C28-C29-C2A |
| 72  | B2    | 501 | 3PE  | C2F-C2G-C2H-C2I |
| 77  | R2    | 601 | NAP  | PN-O3-PA-O1A    |
| 78  | S2    | 401 | PC1  | C32-C31-O31-C3  |
| 72  | B2    | 501 | 3PE  | C3C-C3D-C3E-C3F |
| 73  | 42    | 501 | CDL  | C51-C52-C53-C54 |
| 78  | j2    | 201 | PC1  | C34-C35-C36-C37 |
| 72  | 22    | 401 | 3PE  | O11-C1-C2-C3    |
| 72  | B2    | 501 | 3PE  | O11-C1-C2-C3    |
| 73  | 42    | 501 | CDL  | OB5-CB3-CB4-CB6 |
| 72  | 42    | 502 | 3PE  | C24-C25-C26-C27 |
| 70  | P1    | 301 | HEC  | C3A-C2A-CAA-CBA |
| 73  | 42    | 501 | CDL  | CA3-CA4-CA6-OA8 |
| 72  | 42    | 502 | 3PE  | C26-C27-C28-C29 |
| 72  | 42    | 502 | 3PE  | C29-C2A-C2B-C2C |
| 72  | B2    | 501 | 3PE  | C2-C1-O11-P     |
| 72  | 22    | 401 | 3PE  | C22-C23-C24-C25 |
| 77  | R2    | 601 | NAP  | C3B-C4B-C5B-O5B |
| 72  | 22    | 401 | 3PE  | C2A-C2B-C2C-C2D |
| 72  | 22    | 401 | 3PE  | C25-C26-C27-C28 |
| 78  | S2    | 401 | PC1  | C21-C22-C23-C24 |
| 78  | S2    | 401 | PC1  | C3B-C3C-C3D-C3E |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 77  | R2    | 601 | NAP  | PN-O3-PA-O5B    |
| 74  | 82    | 501 | FMN  | O2'-C2'-C3'-C4' |
| 78  | S2    | 401 | PC1  | C32-C33-C34-C35 |
| 74  | 82    | 501 | FMN  | C1'-C2'-C3'-O3' |
| 78  | j2    | 201 | PC1  | O32-C31-O31-C3  |
| 78  | S2    | 401 | PC1  | O32-C31-O31-C3  |
| 69  | C1    | 402 | HEM  | C2B-C3B-CAB-CBB |
| 72  | 42    | 502 | 3PE  | C3-C2-O21-C21   |
| 73  | 42    | 501 | CDL  | CB3-CB4-OB6-CB5 |
| 73  | 42    | 501 | CDL  | OB5-CB3-CB4-OB6 |
| 78  | S2    | 401 | PC1  | O11-C1-C2-O21   |
| 72  | 42    | 502 | 3PE  | C12-C11-O13-P   |
| 78  | j2    | 201 | PC1  | O21-C2-C3-O31   |
| 78  | S2    | 401 | PC1  | O13-C11-C12-N   |
| 78  | j2    | 201 | PC1  | O13-C11-C12-N   |
| 72  | B2    | 501 | 3PE  | C32-C31-O31-C3  |
| 73  | 42    | 501 | CDL  | OA5-CA3-CA4-CA6 |
| 70  | P1    | 301 | HEC  | C4B-C3B-CAB-CBB |
| 72  | 22    | 401 | 3PE  | O11-C1-C2-O21   |
| 70  | D1    | 301 | HEC  | C1A-C2A-CAA-CBA |
| 72  | 22    | 401 | 3PE  | O21-C2-C3-O31   |
| 72  | 42    | 502 | 3PE  | O21-C2-C3-O31   |
| 72  | B2    | 501 | 3PE  | O32-C31-O31-C3  |
| 72  | 22    | 401 | 3PE  | C1-O11-P-O12    |
| 72  | 22    | 401 | 3PE  | C1-O11-P-O13    |
| 72  | 42    | 502 | 3PE  | C1-O11-P-O12    |
| 72  | 42    | 502 | 3PE  | C1-O11-P-O13    |
| 72  | 42    | 502 | 3PE  | C1-O11-P-O14    |
| 78  | S2    | 401 | PC1  | C1-O11-P-O12    |
| 78  | j2    | 201 | PC1  | C1-O11-P-O14    |
| 72  | 42    | 502 | 3PE  | C27-C28-C29-C2A |
| 73  | 42    | 501 | CDL  | CA4-CA3-OA5-PA1 |
| 78  | j2    | 201 | PC1  | O11-C1-C2-O21   |
| 72  | B2    | 501 | 3PE  | C24-C25-C26-C27 |
| 73  | 42    | 501 | CDL  | C52-C53-C54-C55 |
| 77  | R2    | 601 | NAP  | C3D-C4D-C5D-O5D |
| 70  | D1    | 301 | HEC  | C3A-C2A-CAA-CBA |
| 77  | R2    | 601 | NAP  | C2B-O2B-P2B-O3X |
| 73  | 42    | 501 | CDL  | C14-C15-C16-C17 |
| 73  | 42    | 501 | CDL  | CB4-CB3-OB5-PB2 |
| 72  | 22    | 401 | 3PE  | C26-C27-C28-C29 |
| 70  | D1    | 301 | HEC  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 69  | O1    | 401 | HEM  | CAD-CBD-CGD-O2D |
| 70  | D1    | 301 | HEC  | CAA-CBA-CGA-O2A |
| 70  | P1    | 301 | HEC  | CAA-CBA-CGA-O1A |
| 69  | O1    | 402 | HEM  | CAA-CBA-CGA-O1A |
| 70  | P1    | 301 | HEC  | CAA-CBA-CGA-O2A |
| 69  | C1    | 402 | HEM  | CAD-CBD-CGD-O1D |
| 79  | A3    | 602 | HEA  | CAD-CBD-CGD-O1D |
| 78  | j2    | 201 | PC1  | O21-C21-C22-C23 |
| 69  | C1    | 402 | HEM  | CAA-CBA-CGA-O2A |
| 78  | S2    | 401 | PC1  | C2-C1-O11-P     |
| 69  | O1    | 401 | HEM  | CAD-CBD-CGD-O1D |
| 79  | A3    | 601 | HEA  | CAD-CBD-CGD-O1D |
| 79  | A3    | 602 | HEA  | CAD-CBD-CGD-O2D |
| 70  | P1    | 301 | HEC  | C2A-CAA-CBA-CGA |
| 69  | O1    | 402 | HEM  | CAD-CBD-CGD-O2D |
| 69  | C1    | 401 | HEM  | CAD-CBD-CGD-O1D |
| 72  | B2    | 501 | 3PE  | C2D-C2E-C2F-C2G |
| 69  | C1    | 401 | HEM  | CAD-CBD-CGD-O2D |
| 73  | 42    | 501 | CDL  | C58-C59-C60-C61 |
| 69  | C1    | 402 | HEM  | CAA-CBA-CGA-O1A |
| 69  | C1    | 402 | HEM  | CAD-CBD-CGD-O2D |
| 69  | O1    | 401 | HEM  | CAA-CBA-CGA-O2A |
| 77  | R2    | 601 | NAP  | C4B-C5B-O5B-PA  |
| 72  | 42    | 502 | 3PE  | C2E-C2F-C2G-C2H |
| 72  | B2    | 501 | 3PE  | C32-C33-C34-C35 |
| 72  | 42    | 502 | 3PE  | C1-C2-C3-O31    |
| 69  | O1    | 402 | HEM  | CAA-CBA-CGA-O2A |
| 69  | O1    | 402 | HEM  | CAD-CBD-CGD-O1D |
| 73  | 42    | 501 | CDL  | CA2-C1-CB2-OB2  |
| 79  | A3    | 601 | HEA  | CAD-CBD-CGD-O2D |
| 69  | C1    | 401 | HEM  | CAA-CBA-CGA-O2A |
| 78  | j2    | 201 | PC1  | O22-C21-C22-C23 |
| 72  | B2    | 501 | 3PE  | C26-C27-C28-C29 |
| 72  | B2    | 501 | 3PE  | C38-C39-C3A-C3B |
| 69  | O1    | 401 | HEM  | CAA-CBA-CGA-O1A |
| 79  | A3    | 601 | HEA  | CAA-CBA-CGA-O1A |
| 72  | B2    | 501 | 3PE  | C25-C26-C27-C28 |
| 72  | B2    | 501 | 3PE  | C1-C2-C3-O31    |
| 69  | C1    | 402 | HEM  | C4B-C3B-CAB-CBB |
| 79  | A3    | 602 | HEA  | CAA-CBA-CGA-O2A |
| 69  | C1    | 401 | HEM  | CAA-CBA-CGA-O1A |
| 73  | 42    | 501 | CDL  | C71-C72-C73-C74 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 72  | B2    | 501 | 3PE  | O21-C2-C3-O31   |
| 79  | A3    | 602 | HEA  | CAA-CBA-CGA-O1A |
| 78  | S2    | 401 | PC1  | C23-C24-C25-C26 |
| 78  | S2    | 401 | PC1  | C26-C27-C28-C29 |
| 74  | 82    | 501 | FMN  | O2'-C2'-C3'-O3' |
| 72  | 42    | 502 | 3PE  | C2B-C2C-C2D-C2E |
| 72  | B2    | 501 | 3PE  | C3B-C3C-C3D-C3E |
| 79  | A3    | 602 | HEA  | C26-C15-C16-C17 |
| 73  | 42    | 501 | CDL  | C76-C77-C78-C79 |
| 78  | j2    | 201 | PC1  | O11-C1-C2-C3    |
| 79  | A3    | 601 | HEA  | CAA-CBA-CGA-O2A |
| 78  | S2    | 401 | PC1  | O21-C21-C22-C23 |
| 70  | P1    | 301 | HEC  | CAD-CBD-CGD-O2D |
| 78  | j2    | 201 | PC1  | O31-C31-C32-C33 |
| 78  | j2    | 201 | PC1  | C3A-C3B-C3C-C3D |
| 78  | j2    | 201 | PC1  | O32-C31-C32-C33 |
| 78  | S2    | 401 | PC1  | O22-C21-C22-C23 |

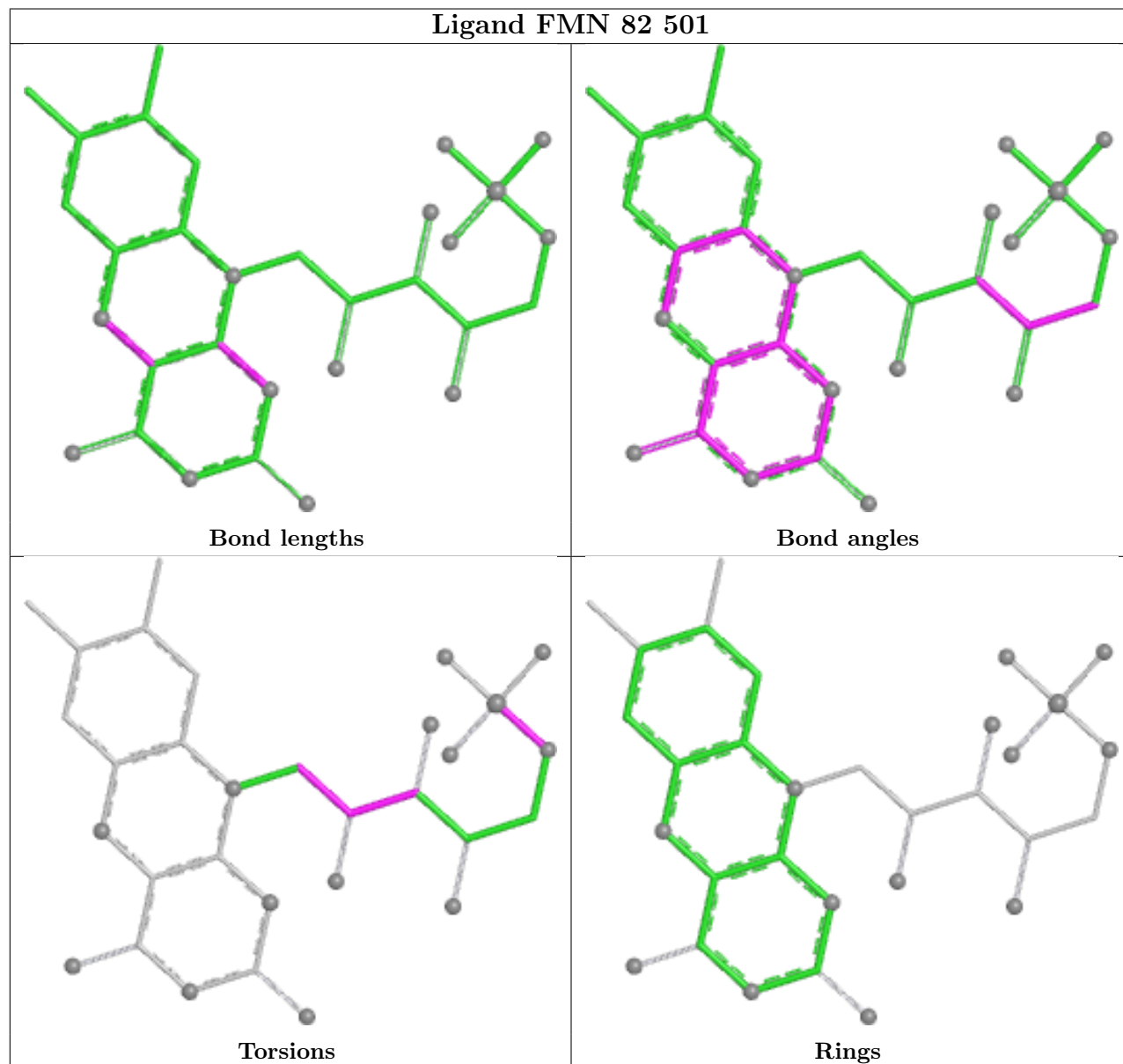
There are no ring outliers.

17 monomers are involved in 82 short contacts:

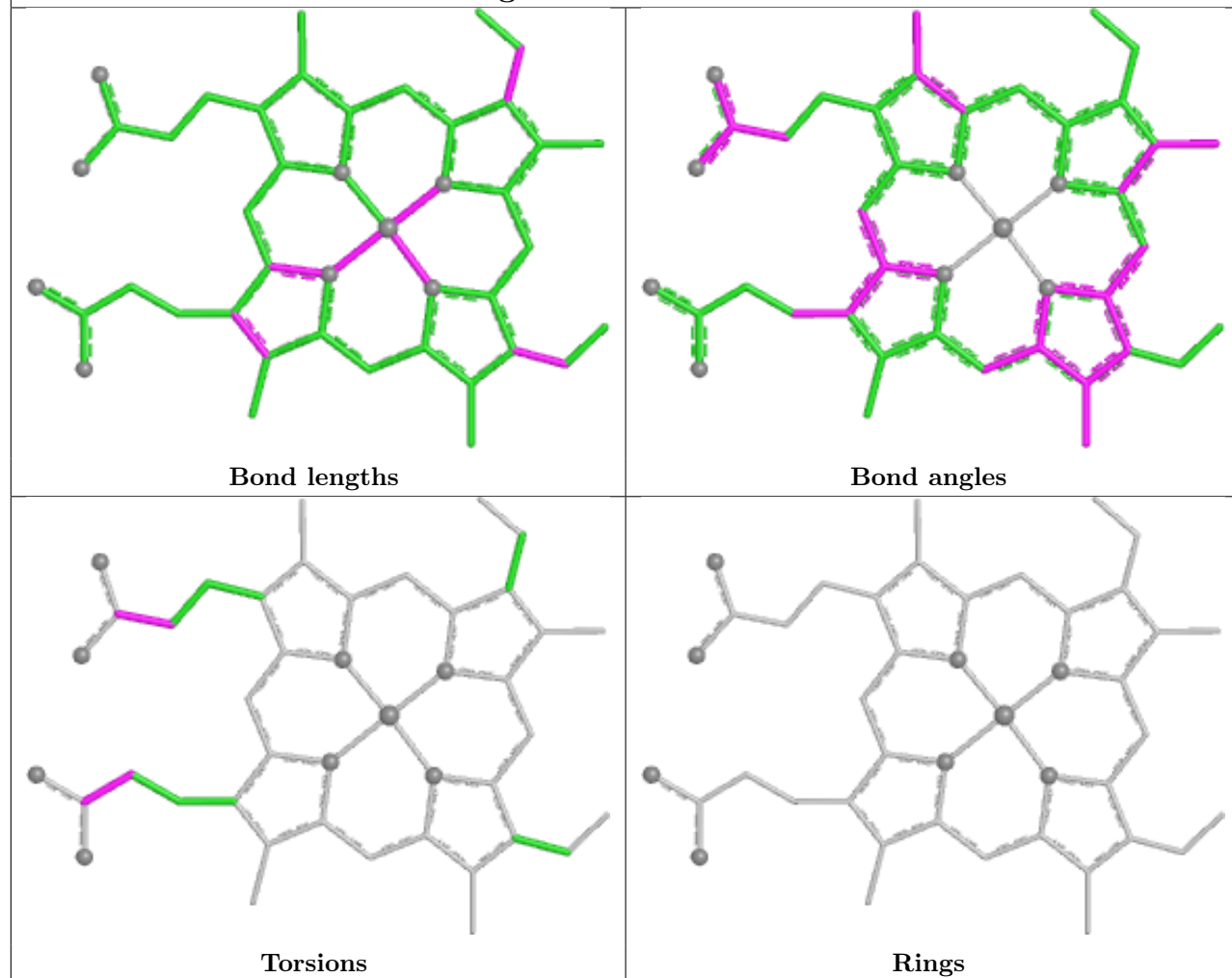
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 74  | 82    | 501 | FMN  | 2       | 0            |
| 69  | O1    | 402 | HEM  | 14      | 0            |
| 69  | C1    | 402 | HEM  | 13      | 0            |
| 72  | 42    | 502 | 3PE  | 1       | 0            |
| 70  | P1    | 301 | HEC  | 5       | 0            |
| 78  | j2    | 201 | PC1  | 1       | 0            |
| 72  | B2    | 501 | 3PE  | 1       | 0            |
| 75  | A2    | 801 | SF4  | 4       | 0            |
| 75  | A2    | 802 | SF4  | 8       | 0            |
| 70  | D1    | 301 | HEC  | 5       | 0            |
| 79  | A3    | 601 | HEA  | 1       | 0            |
| 69  | O1    | 401 | HEM  | 11      | 0            |
| 69  | C1    | 401 | HEM  | 5       | 0            |
| 73  | 42    | 501 | CDL  | 2       | 0            |
| 77  | R2    | 601 | NAP  | 3       | 0            |
| 72  | 22    | 401 | 3PE  | 3       | 0            |
| 79  | A3    | 602 | HEA  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

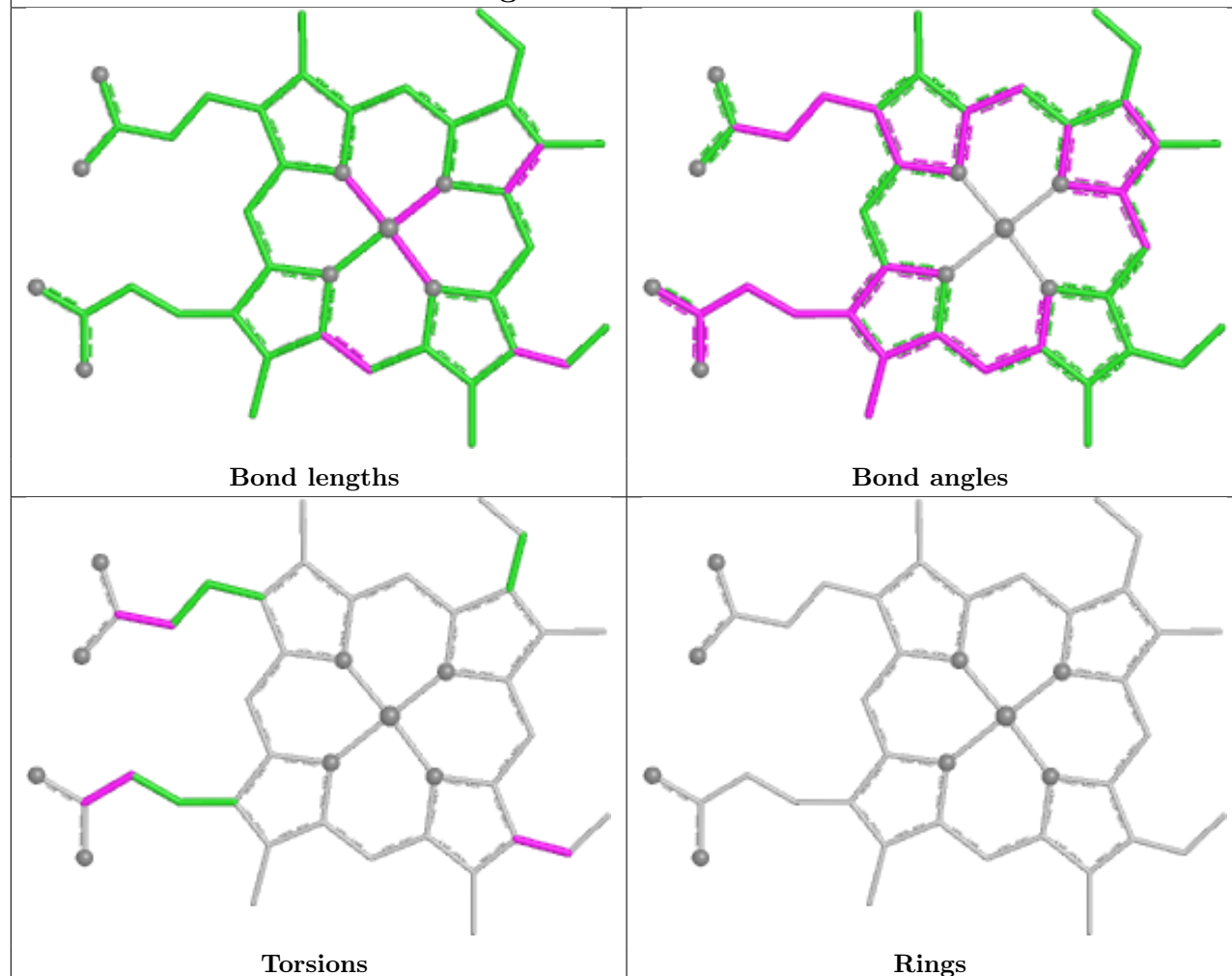
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



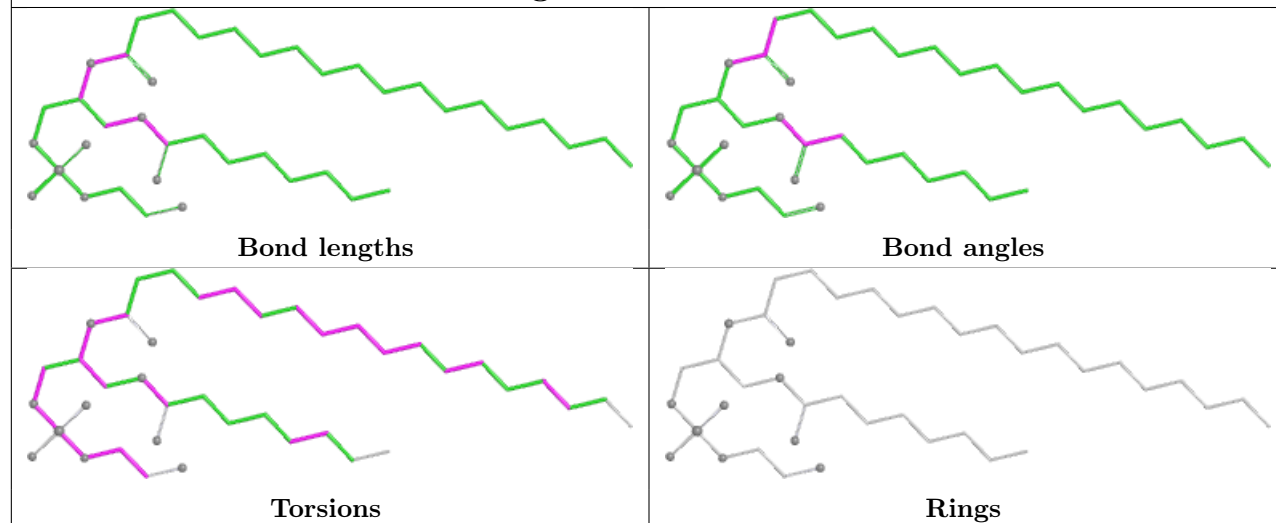
## Ligand HEM O1 402



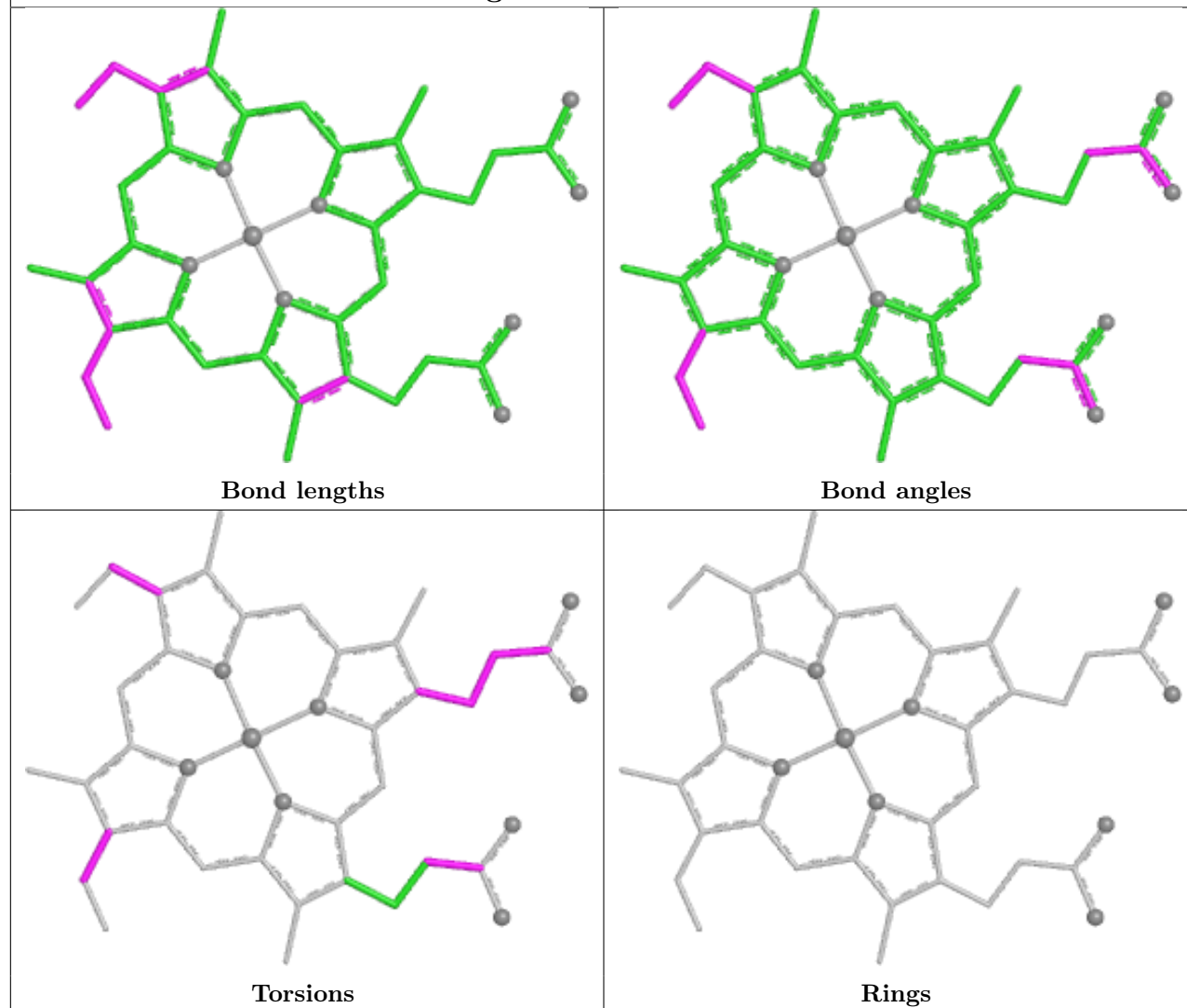
## Ligand HEM C1 402



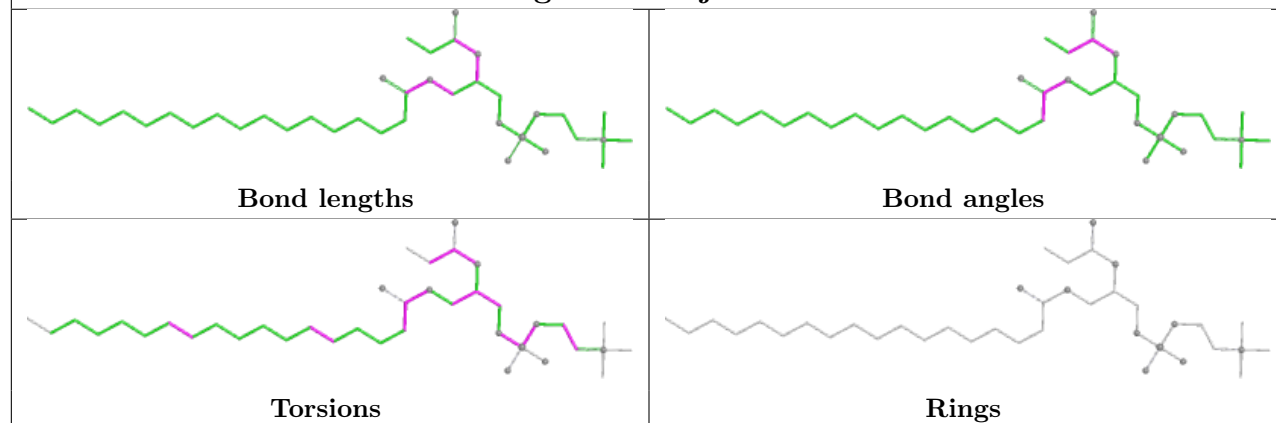
## Ligand 3PE 42 502

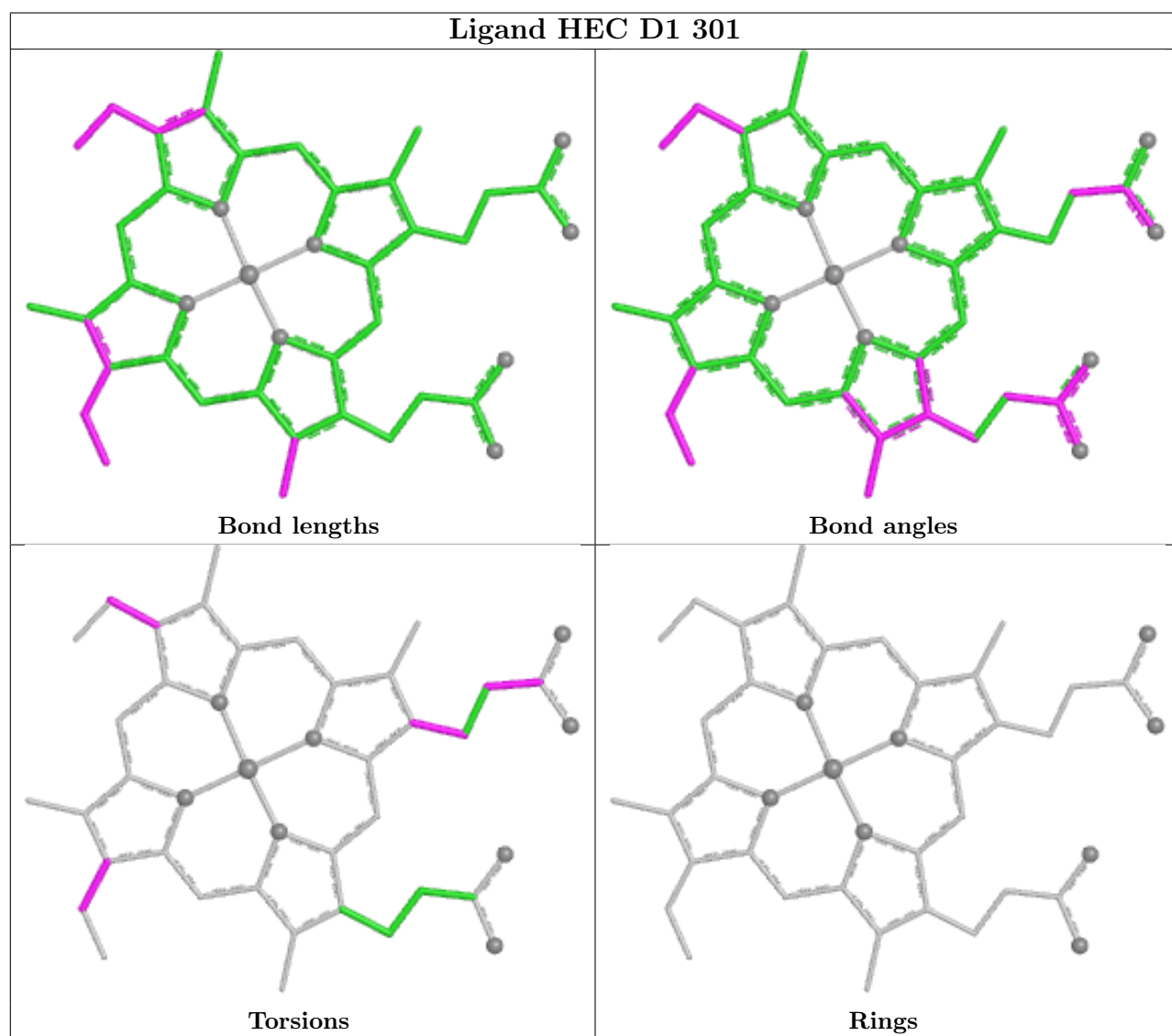
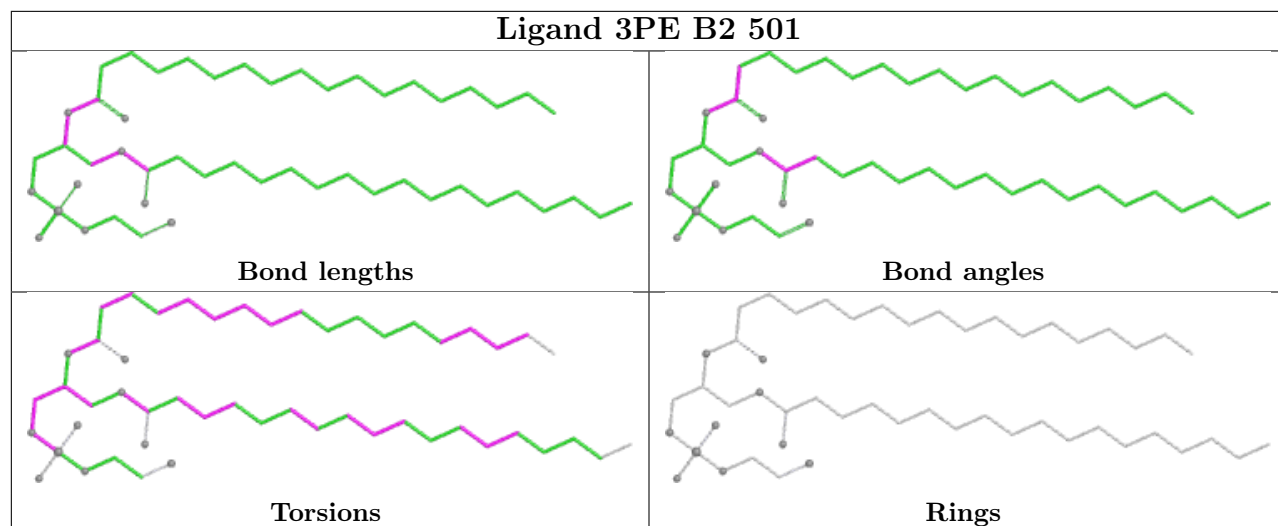


## Ligand HEC P1 301

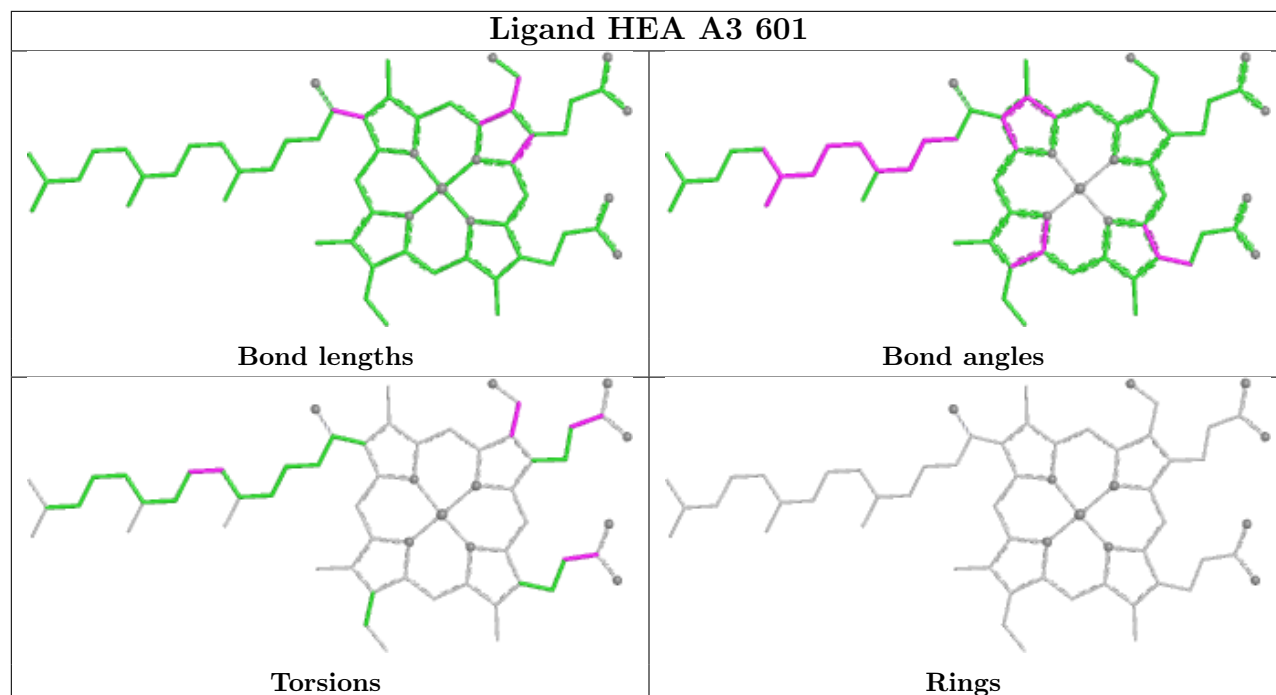


## Ligand PC1 j2 201

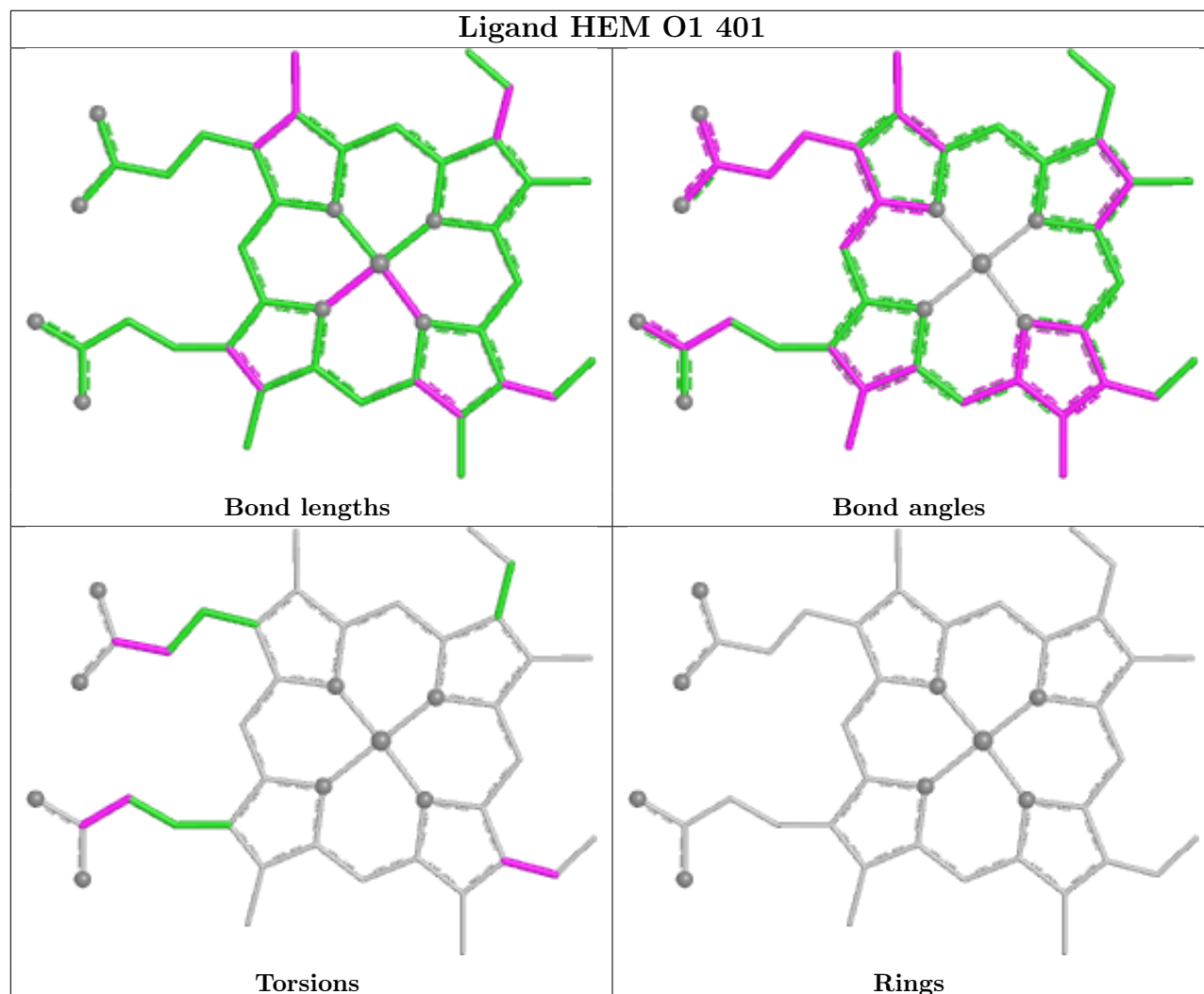




## Ligand HEA A3 601

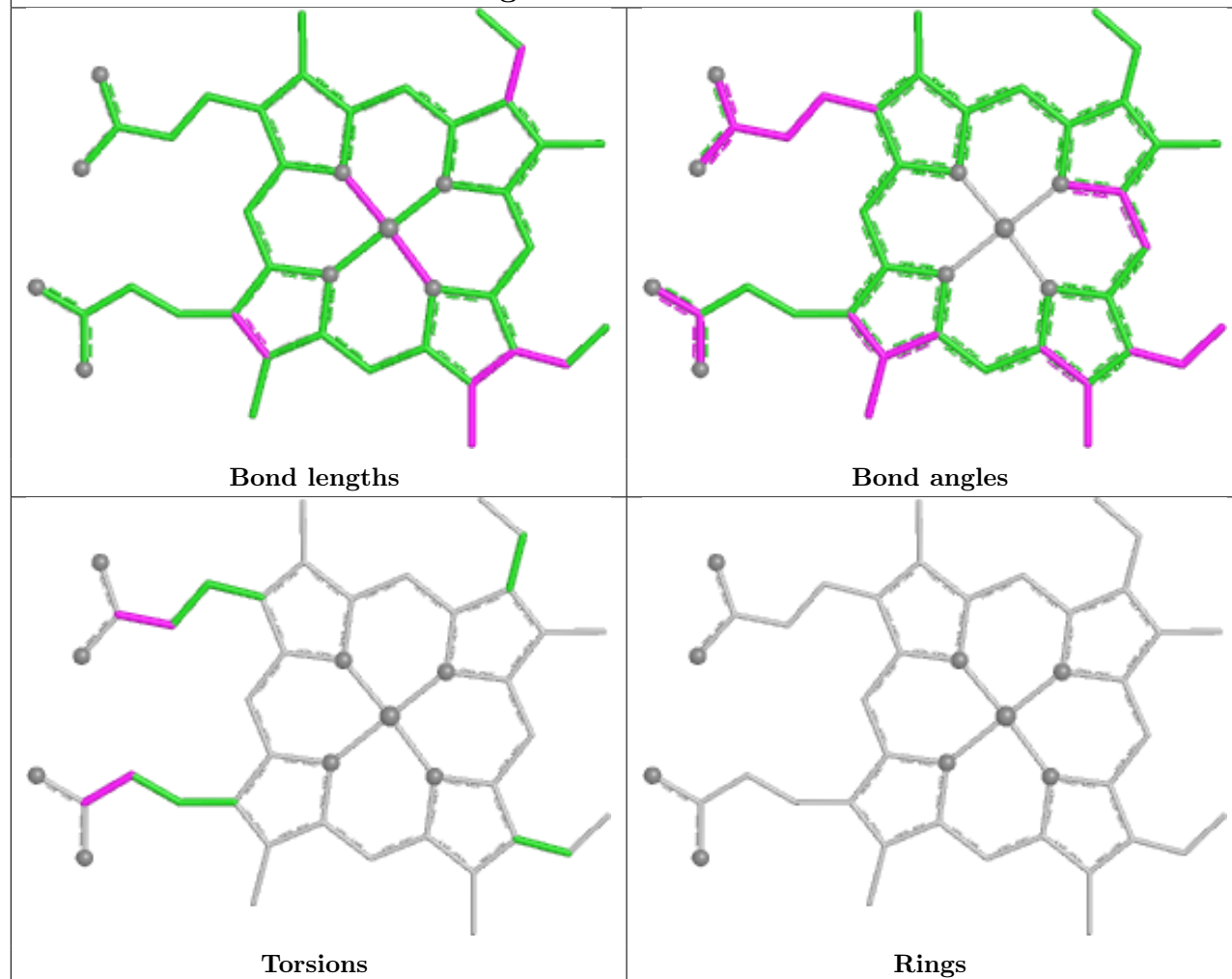


## Ligand HEM O1 401

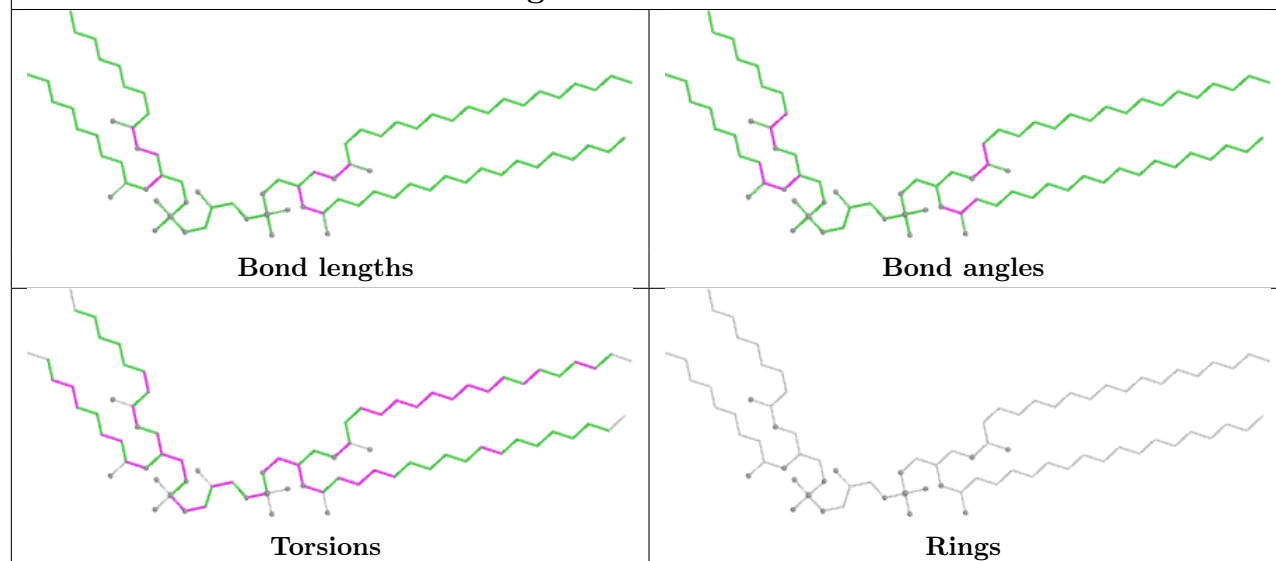


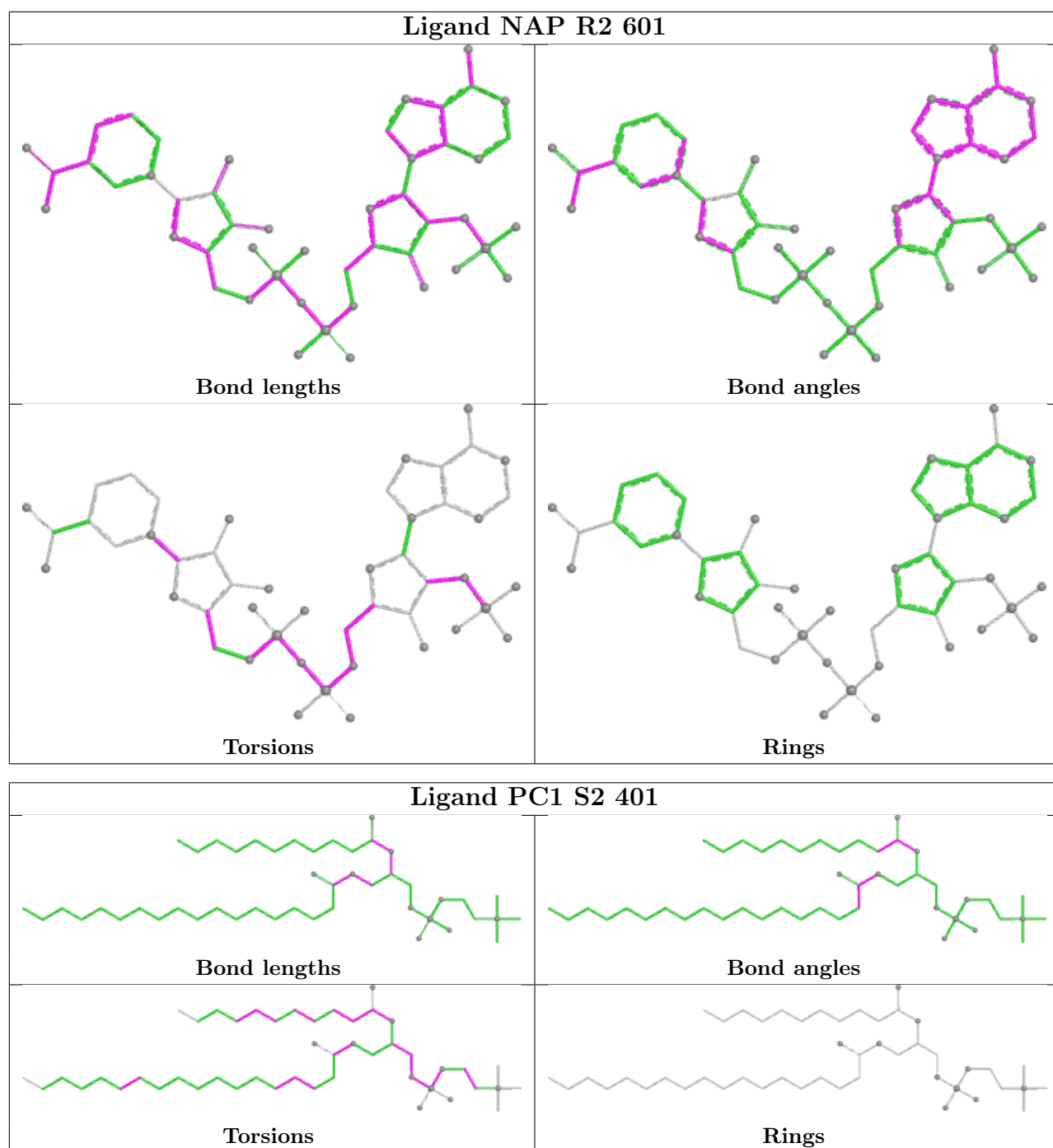


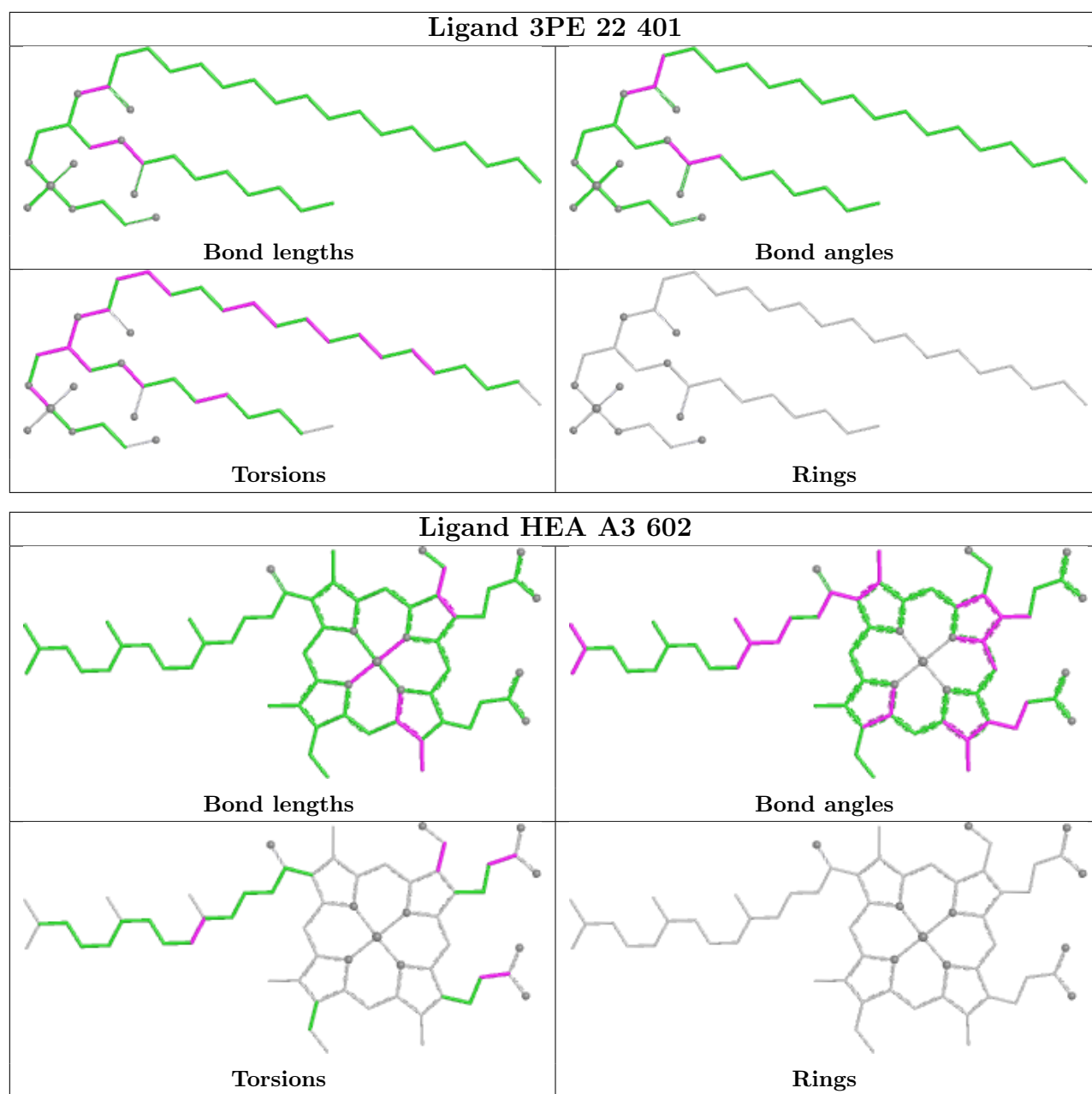
## Ligand HEM C1 401



## Ligand CDL 42 501







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

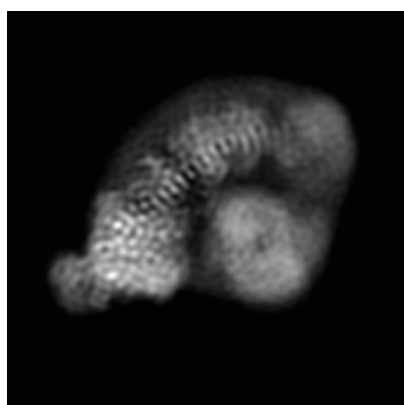
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30706. These allow visual inspection of the internal detail of the map and identification of artifacts.

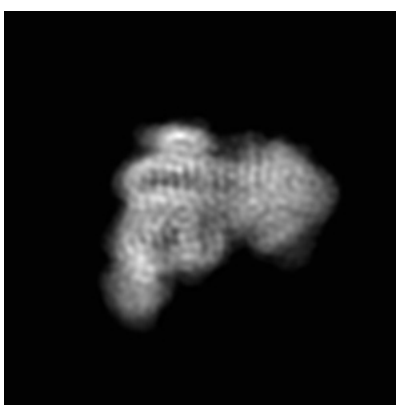
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

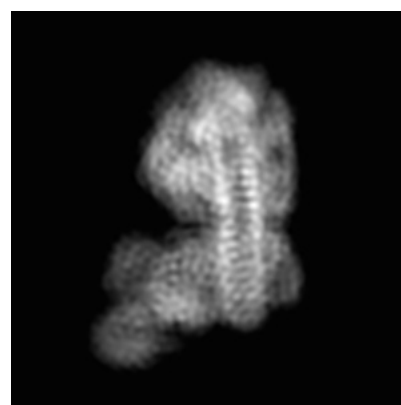
#### 6.1.1 Primary map



X



Y

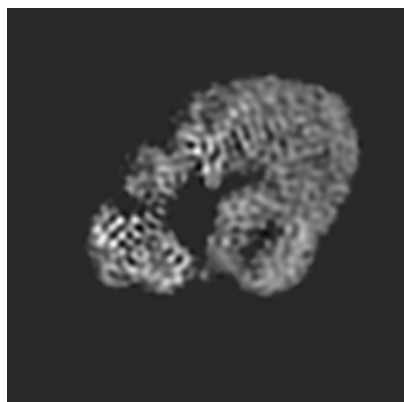


Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 140



Y Index: 140

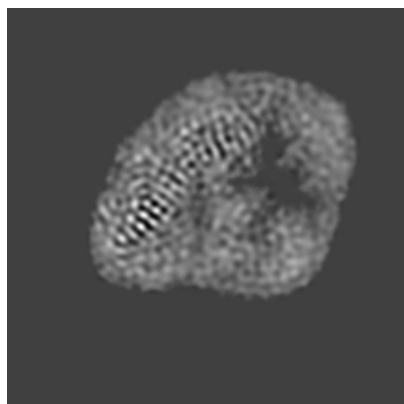


Z Index: 140

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

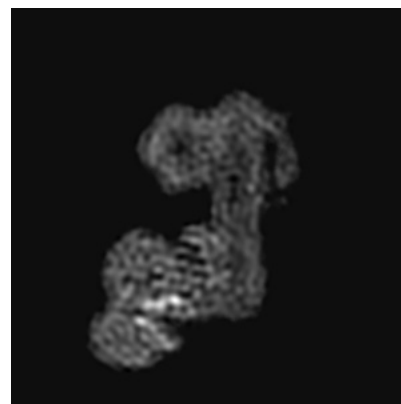
### 6.3.1 Primary map



X Index: 149



Y Index: 79



Z Index: 95

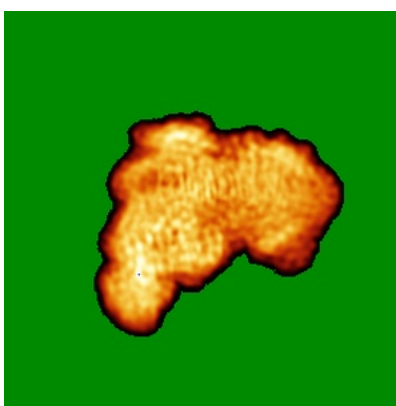
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

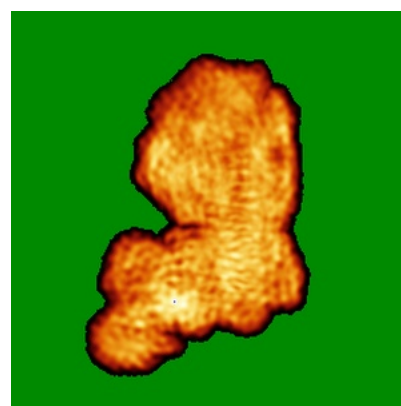
### 6.4.1 Primary map



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.

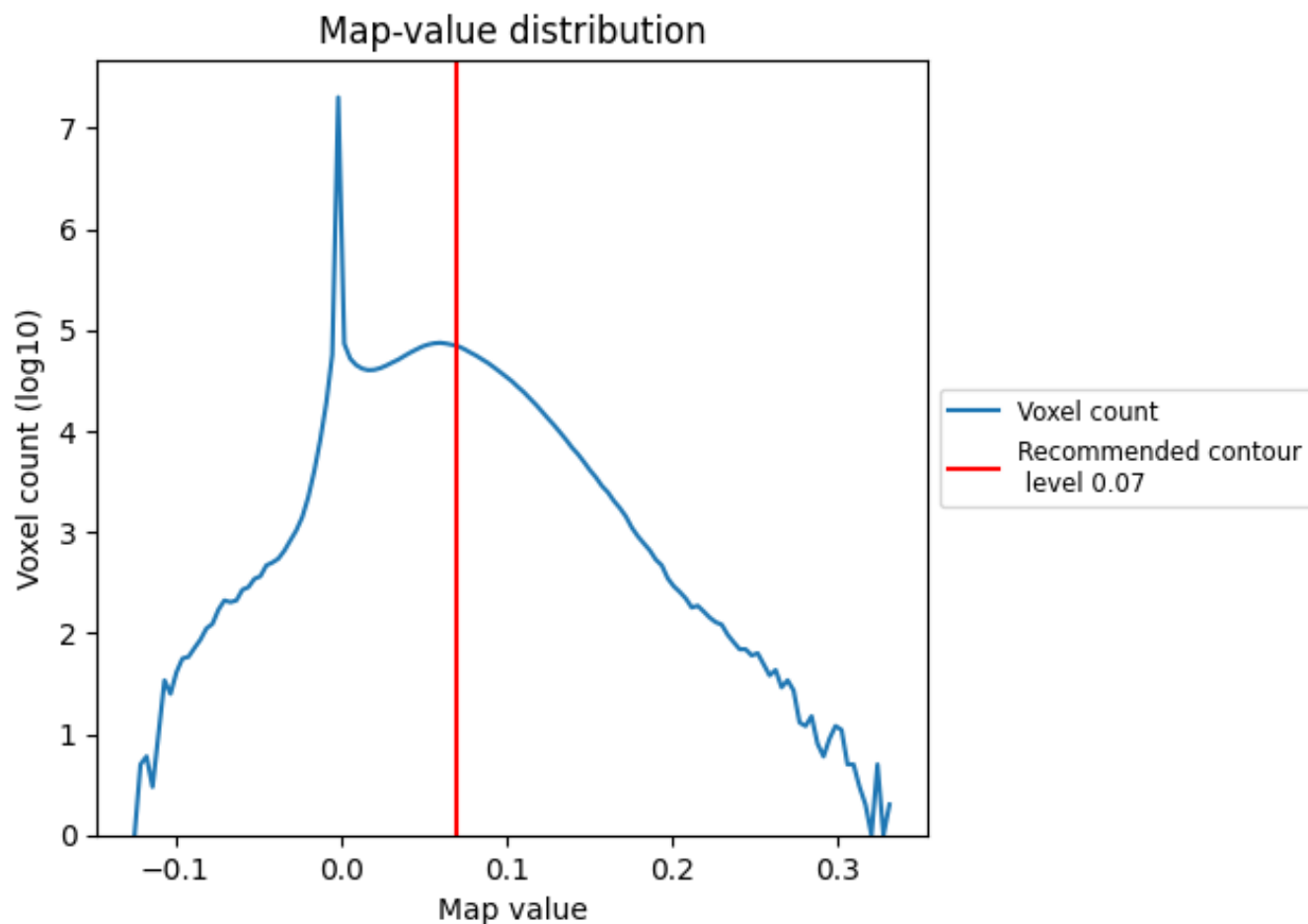
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

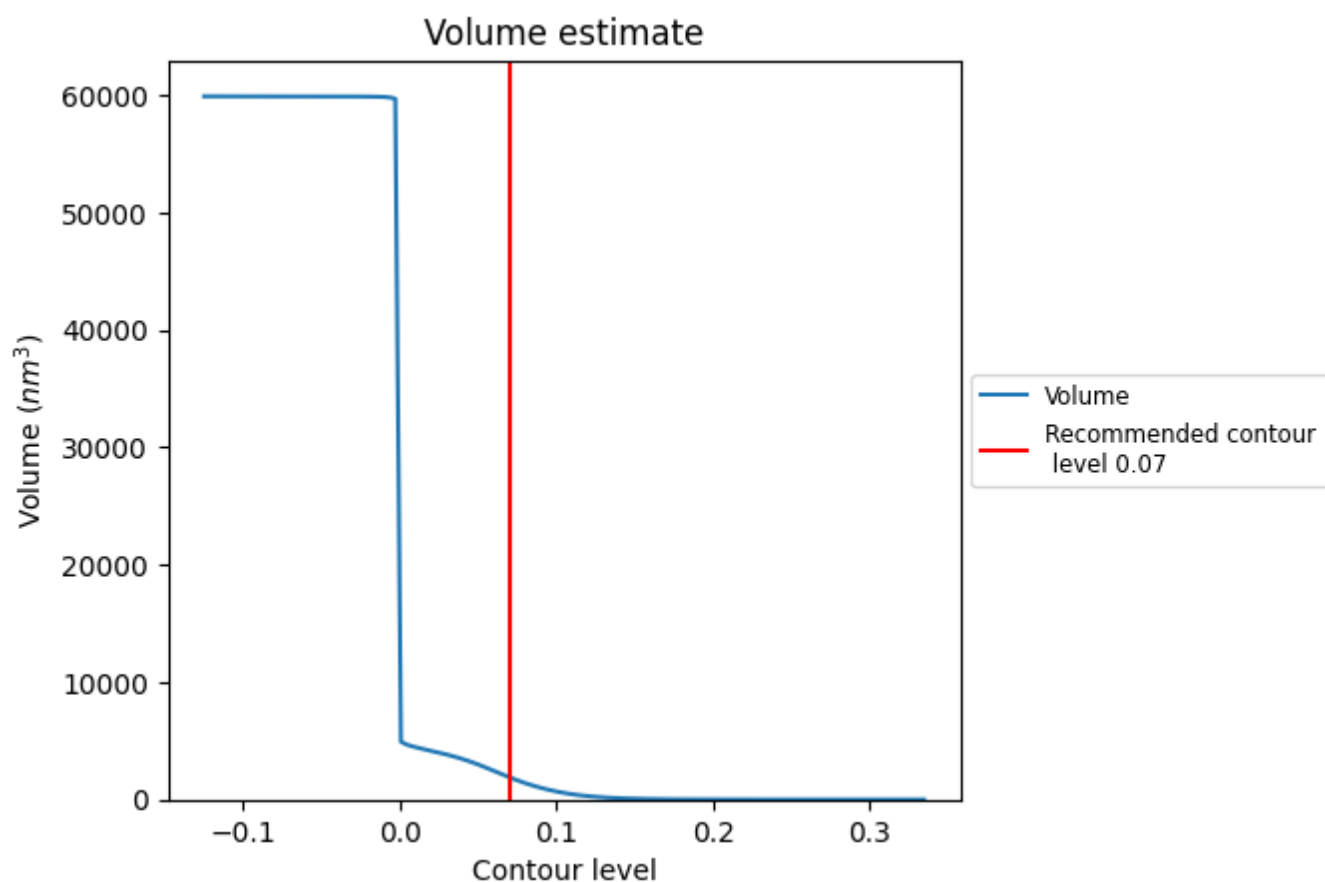
This section contains the results of statistical analysis of the map.

### 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](#)

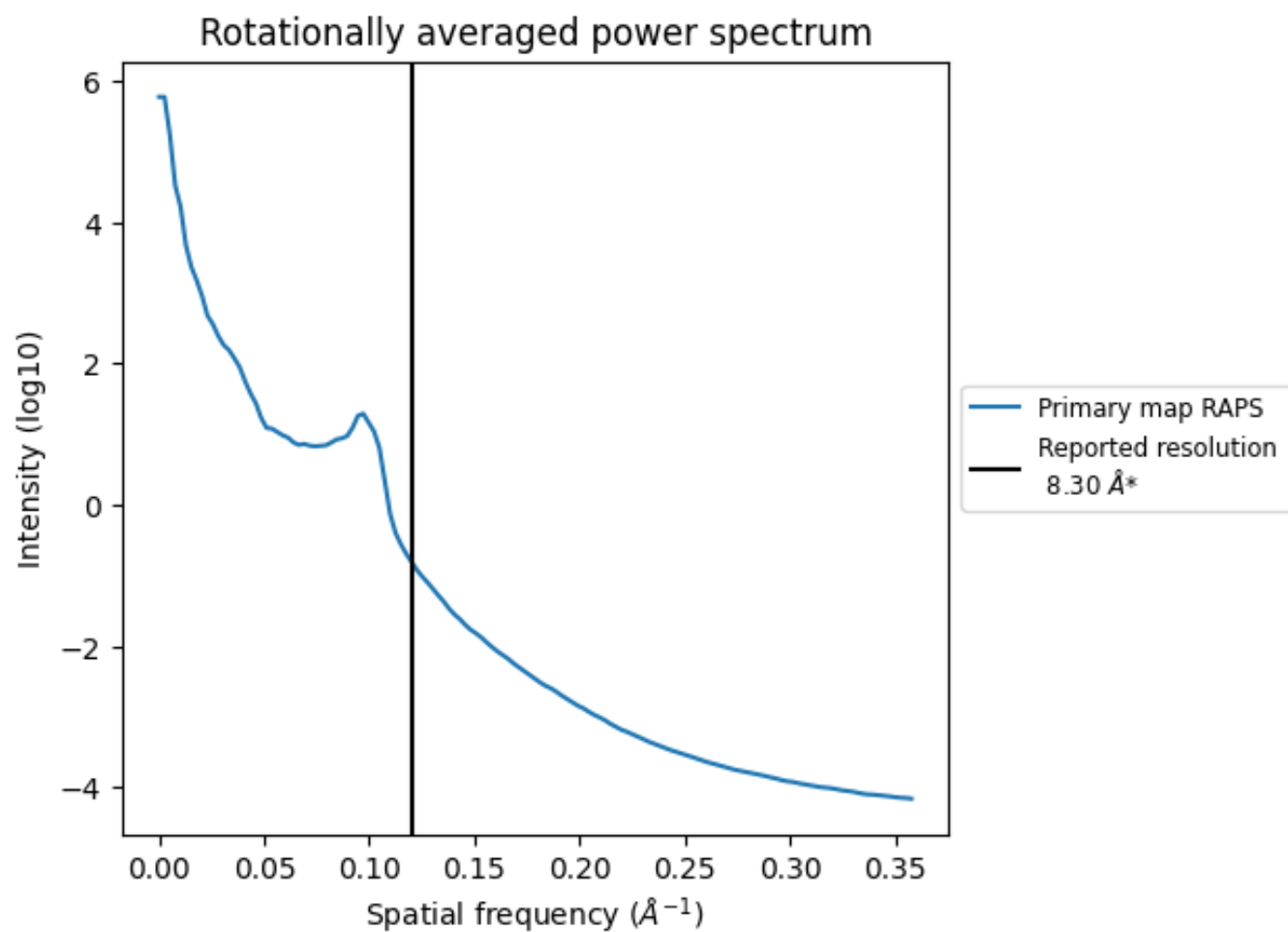


The volume at the recommended contour level is 1904 nm<sup>3</sup>; this corresponds to an approximate mass of 1720 kDa.

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 0.120 Å<sup>-1</sup>

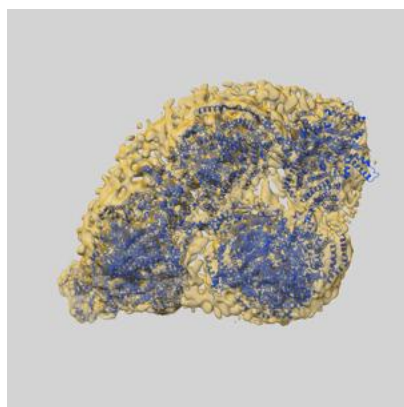
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

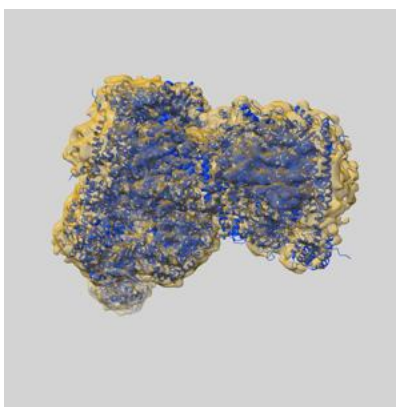
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30706 and PDB model 7DKF. Per-residue inclusion information can be found in section [3](#) on page [25](#).

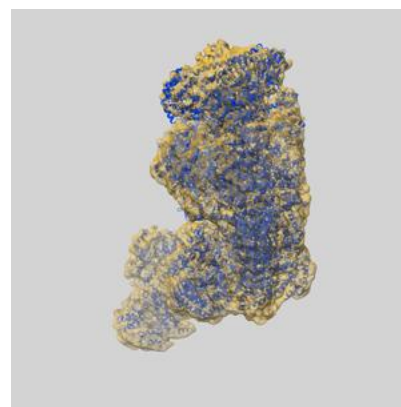
### 9.1 Map-model overlay [i](#)



X



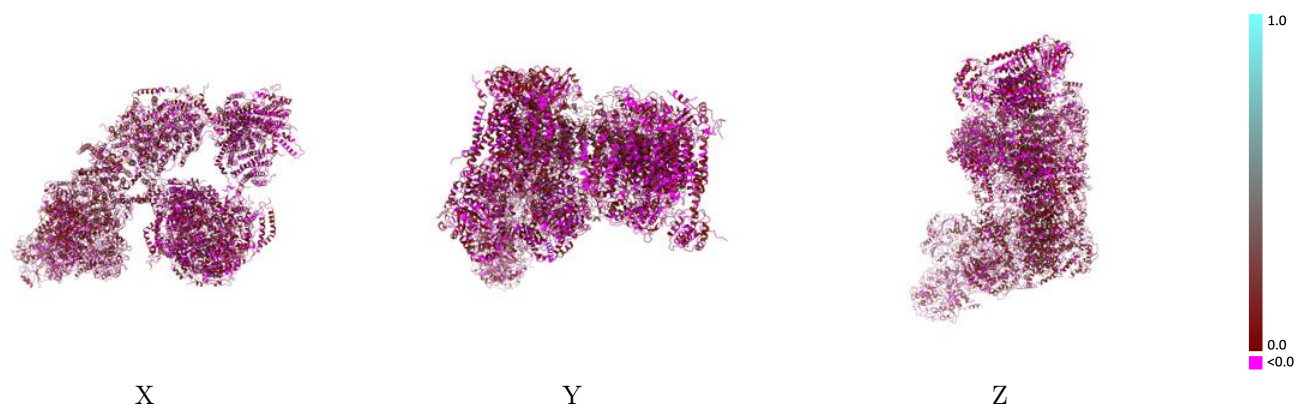
Y



Z

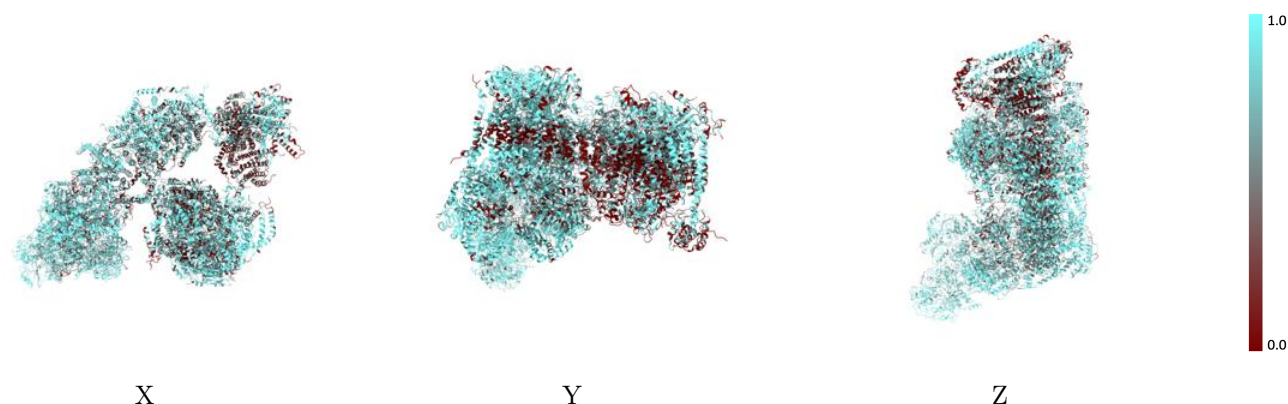
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



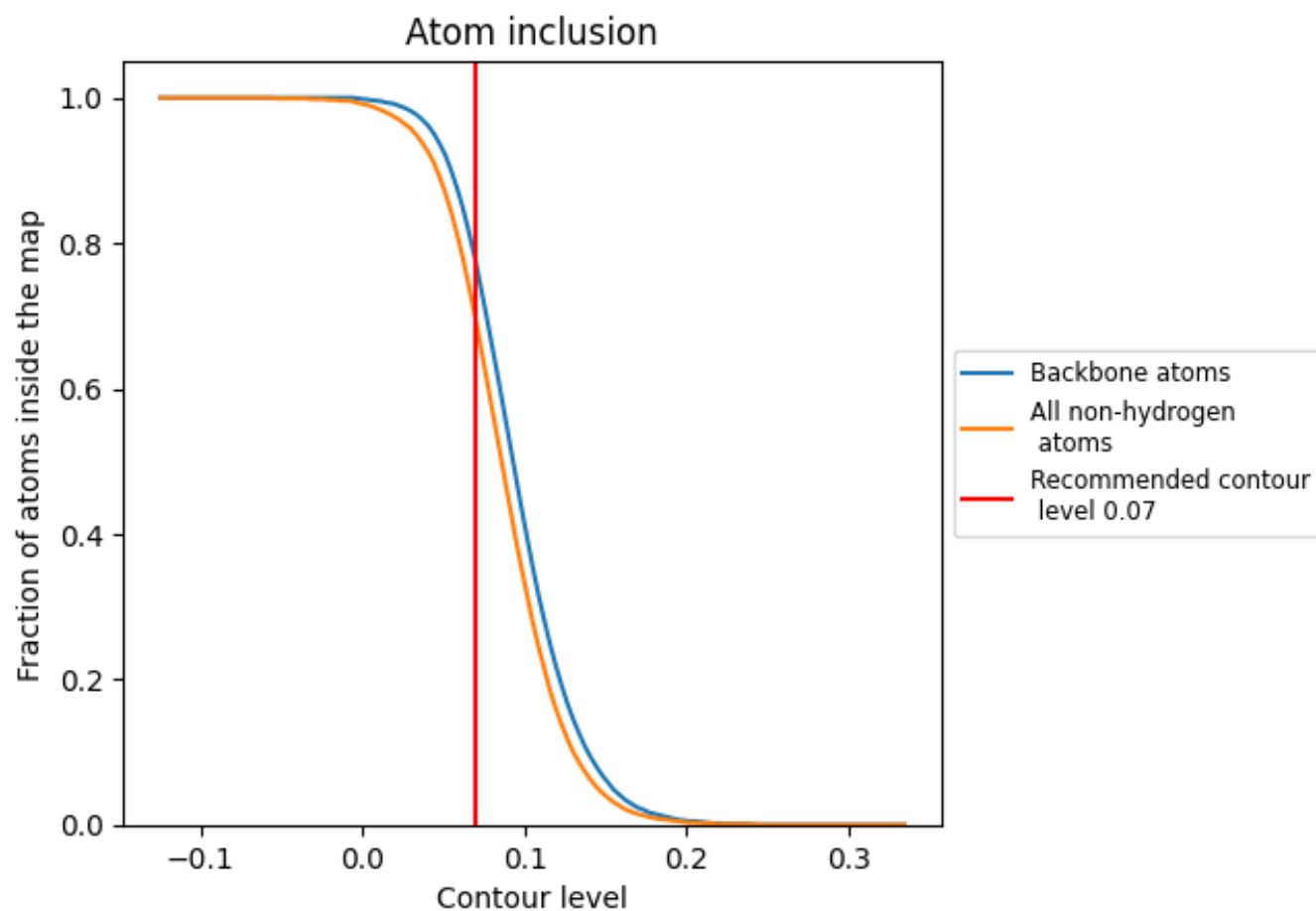
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 69% 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   |  0.6940   |  0.0740    |
| 12    |  0.6860   |  0.0940    |
| 22    |  0.6830   |  0.1120    |
| 32    |  0.6530   |  0.1220    |
| 42    |  0.6360   |  0.0960    |
| 52    |  0.7230   |  0.1370    |
| 62    |  0.5780   |  0.0660    |
| 72    |  0.6180   |  0.1000    |
| 82    |  0.9020   |  0.0870    |
| 92    |  0.8570   |  0.0660    |
| A1    |  0.8310   |  0.0620    |
| A2    |  0.8730   |  0.0890    |
| A3    |  0.4940   |  0.0340    |
| B1    |  0.8390   |  0.0590    |
| B2    |  0.7920  |  0.0930   |
| B3    |  0.6750 |  0.0240  |
| C1    |  0.6440 |  0.0780  |
| C2    |  0.7840 |  0.0880  |
| C3    |  0.3640 |  0.0330  |
| D1    |  0.8390 |  0.0660  |
| D2    |  0.7750 |  0.0850  |
| D3    |  0.4080 |  0.0180  |
| E1    |  0.6030 |  0.0280  |
| E2    |  0.8570 |  0.0840  |
| E3    |  0.4270 |  0.0480  |
| F1    |  0.7560 |  0.0750  |
| F2    |  0.8600 |  0.1250  |
| F3    |  0.3470 |  0.0430  |
| G1    |  0.6280 |  0.0510  |
| G2    |  0.7500 |  0.0850  |
| G3    |  0.2610 |  0.0210  |
| H1    |  0.8150 |  0.0760  |
| H2    |  0.8520 |  0.1200  |
| H3    |  0.4570 |  0.0170  |
| I1    |  0.3710 |  -0.0560 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| I2    |  0.6500   |  0.0530    |
| I3    |  0.6620   |  0.0800    |
| J1    |  0.6190   |  0.0260    |
| J2    |  0.8410   |  0.1030    |
| J3    |  0.2490   |  0.0540    |
| K1    |  0.6160   |  0.0770    |
| K2    |  0.9020   |  0.1150    |
| K3    |  0.5650   |  0.0470    |
| L2    |  0.7600   |  0.1050    |
| L3    |  0.4180   |  0.0440    |
| M1    |  0.6890   |  0.0380    |
| M2    |  0.6580   |  0.1210    |
| M3    |  0.4820   |  0.1140    |
| N1    |  0.7870   |  0.0460    |
| N2    |  0.8970   |  0.1390    |
| O1    |  0.5690   |  0.0530    |
| O2    |  0.7560   |  0.1220    |
| P1    |  0.7400   |  0.0410    |
| P2    |  0.7500   |  0.1080    |
| Q1    |  0.6350  |  0.0400   |
| Q2    |  0.8640 |  0.1250  |
| R1    |  0.5960 |  0.0680  |
| R2    |  0.7930 |  0.0950  |
| S1    |  0.4540 |  0.0610  |
| S2    |  0.5560 |  0.1020  |
| T1    |  0.6370 |  0.0660  |
| T2    |  0.5780 |  0.1090  |
| U1    |  0.3420 |  -0.0100 |
| U2    |  0.5780 |  0.0750  |
| V1    |  0.4770 |  0.0600  |
| V2    |  0.8740 |  0.1340  |
| W1    |  0.3020 |  0.0720  |
| W2    |  0.6500 |  0.0430  |
| X2    |  0.8470 |  0.1100  |
| Y2    |  0.7370 |  0.0930  |
| Z2    |  0.6530 |  0.0540  |
| a2    |  0.5460 |  0.0940  |
| b2    |  0.8980 |  0.1150  |
| c2    |  0.8810 |  0.1120  |
| d2    |  0.7520 |  0.0280  |
| e2    |  0.6240 |  0.0750  |
| f2    |  0.6410 |  0.0690  |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| g2    |  0.8340 |  0.0960 |
| h2    |  0.7420 |  0.1060 |
| i2    |  0.8430 |  0.1620 |
| j2    |  0.8470 |  0.1310 |