



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:03 PM UTC

PDB ID : 5FLC / pdb\_00005flc  
EMDB ID : EMD-3213  
Title : Architecture of human mTOR Complex 1 - 5.9 Angstrom reconstruction  
Authors : Aylett, C.H.S.; Sauer, E.; Imseng, S.; Boehringer, D.; Hall, M.N.; Ban, N.; Maier, T.  
Deposited on : 2015-10-23  
Resolution : 5.90 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

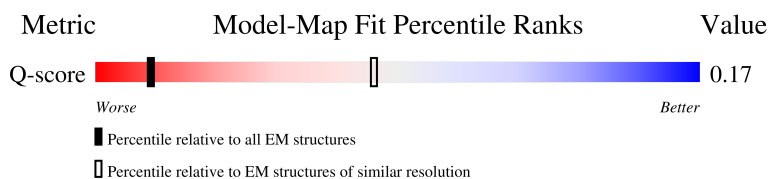
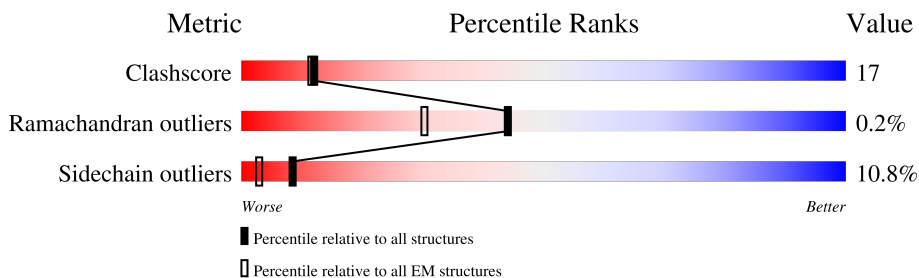
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.90 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                       | 501 ( 5.40 - 6.40 )                                      |

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   | 1     | 615    | <div> <div>57%</div> <div> <div></div> <div>62%</div> <div>38%</div> </div> </div> |
| 1   | 3     | 615    | <div> <div>57%</div> <div> <div></div> <div>62%</div> <div>38%</div> </div> </div> |
| 2   | 2     | 365    | <div> <div>6%</div> <div> <div></div> <div>57%</div> <div>43%</div> </div> </div>  |
| 2   | 4     | 365    | <div> <div>6%</div> <div> <div></div> <div>58%</div> <div>42%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | A     | 1029   |                  |
| 3   | E     | 1029   |                  |
| 4   | B     | 1168   |                  |
| 4   | F     | 1168   |                  |
| 5   | C     | 107    |                  |
| 5   | G     | 107    |                  |
| 6   | D     | 326    |                  |
| 6   | H     | 326    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 7   | RAP  | C     | 999 | X         | -        | -       | -                |
| 7   | RAP  | G     | 999 | X         | -        | -       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47536 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 SERINE/THREONINE-PROTEIN KINASE MTOR.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 1   | 1     | 615      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3690  | 2460 | 615 | 615 |         |       |
| 1   | 3     | 615      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3690  | 2460 | 615 | 615 |         |       |

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 2   | 2     | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2190  | 1460 | 365 | 365 |         |       |
| 2   | 4     | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2190  | 1460 | 365 | 365 |         |       |

- Molecule 3 is a protein called REGULATORY-ASSOCIATED PROTEIN OF MTOR.

| Mol | Chain | Residues | Atoms |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 3   | A     | 1029     | Total | C    | N    | O    | 0       | 0     |
|     |       |          | 6174  | 4116 | 1029 | 1029 |         |       |
| 3   | E     | 1029     | Total | C    | N    | O    | 0       | 0     |
|     |       |          | 6174  | 4116 | 1029 | 1029 |         |       |

- Molecule 4 is a protein called SERINE/THREONINE-PROTEIN KINASE MTOR.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | B     | 1050     | Total | C    | N    | O    | S  | 1       | 0     |
|     |       |          | 8551  | 5439 | 1506 | 1544 | 62 |         |       |
| 4   | F     | 1050     | Total | C    | N    | O    | S  | 1       | 0     |
|     |       |          | 8551  | 5439 | 1506 | 1544 | 62 |         |       |

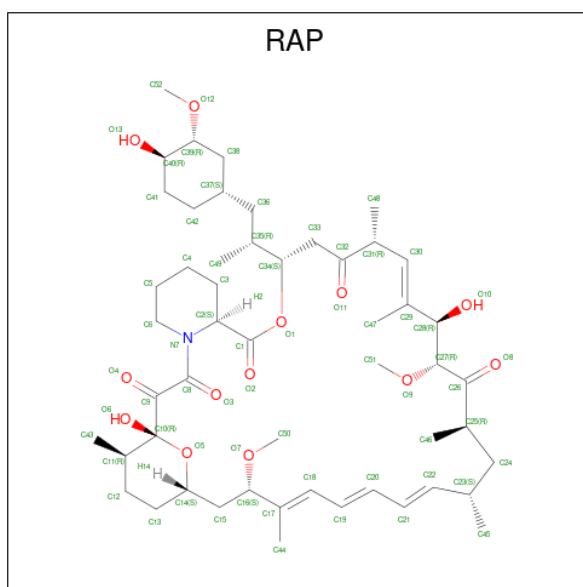
- Molecule 5 is a protein called FKBP.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5   | C     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 642   | 428 | 107 | 107 |         |       |
| 5   | G     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 642   | 428 | 107 | 107 |         |       |

- Molecule 6 is a protein called TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | D     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2456  | 1526 | 436 | 476 | 18 |         |       |
| 6   | H     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2456  | 1526 | 436 | 476 | 18 |         |       |

- Molecule 7 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (CCD ID: RAP) (formula:  $C_{51}H_{79}NO_{13}$ ).

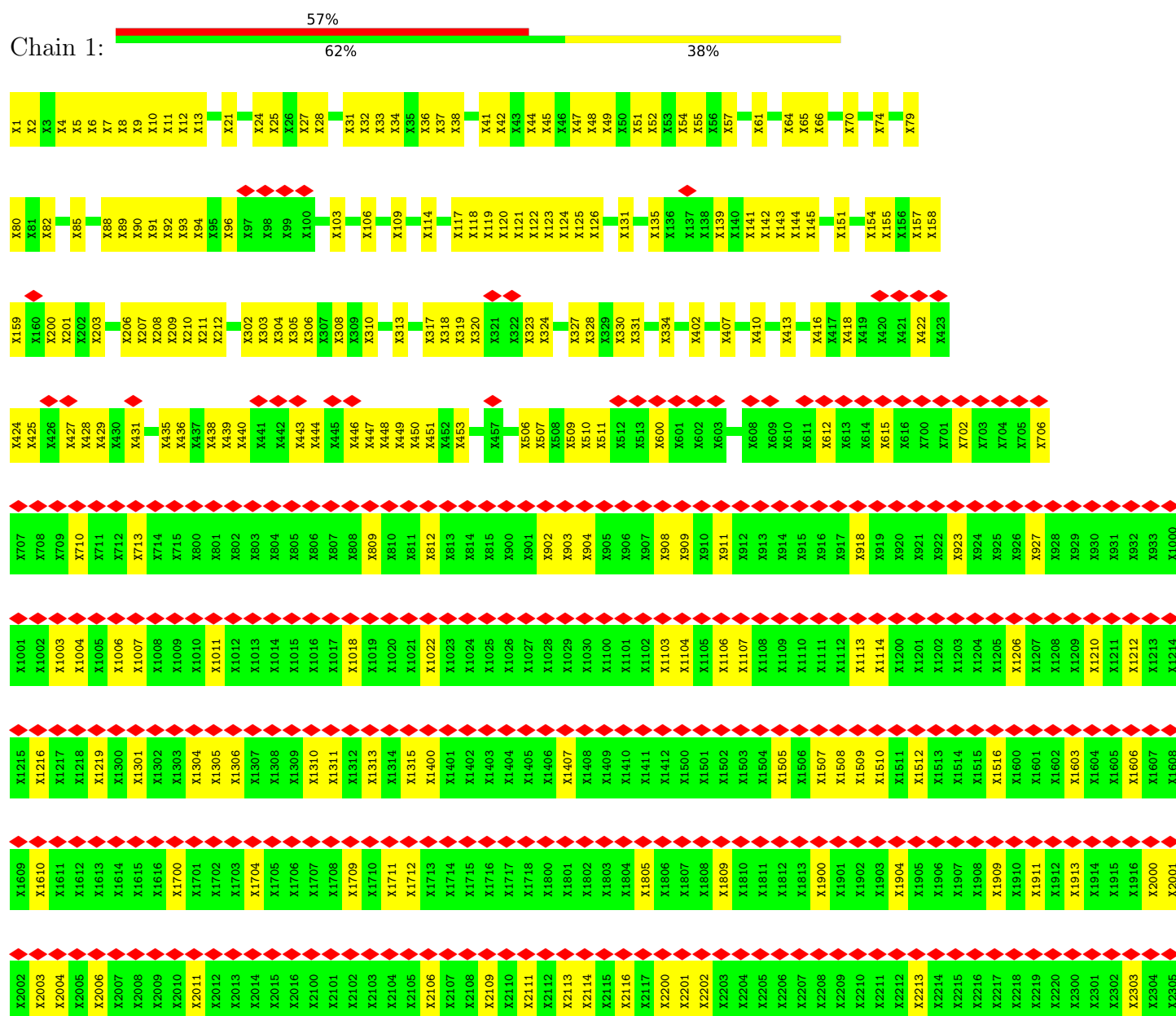


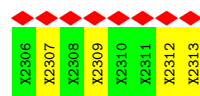
| Mol | Chain | Residues | Atoms |    |   |    | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 7   | C     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 65    | 51 | 1 | 13 |         |
| 7   | G     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 65    | 51 | 1 | 13 |         |

### 3 Residue-property plots

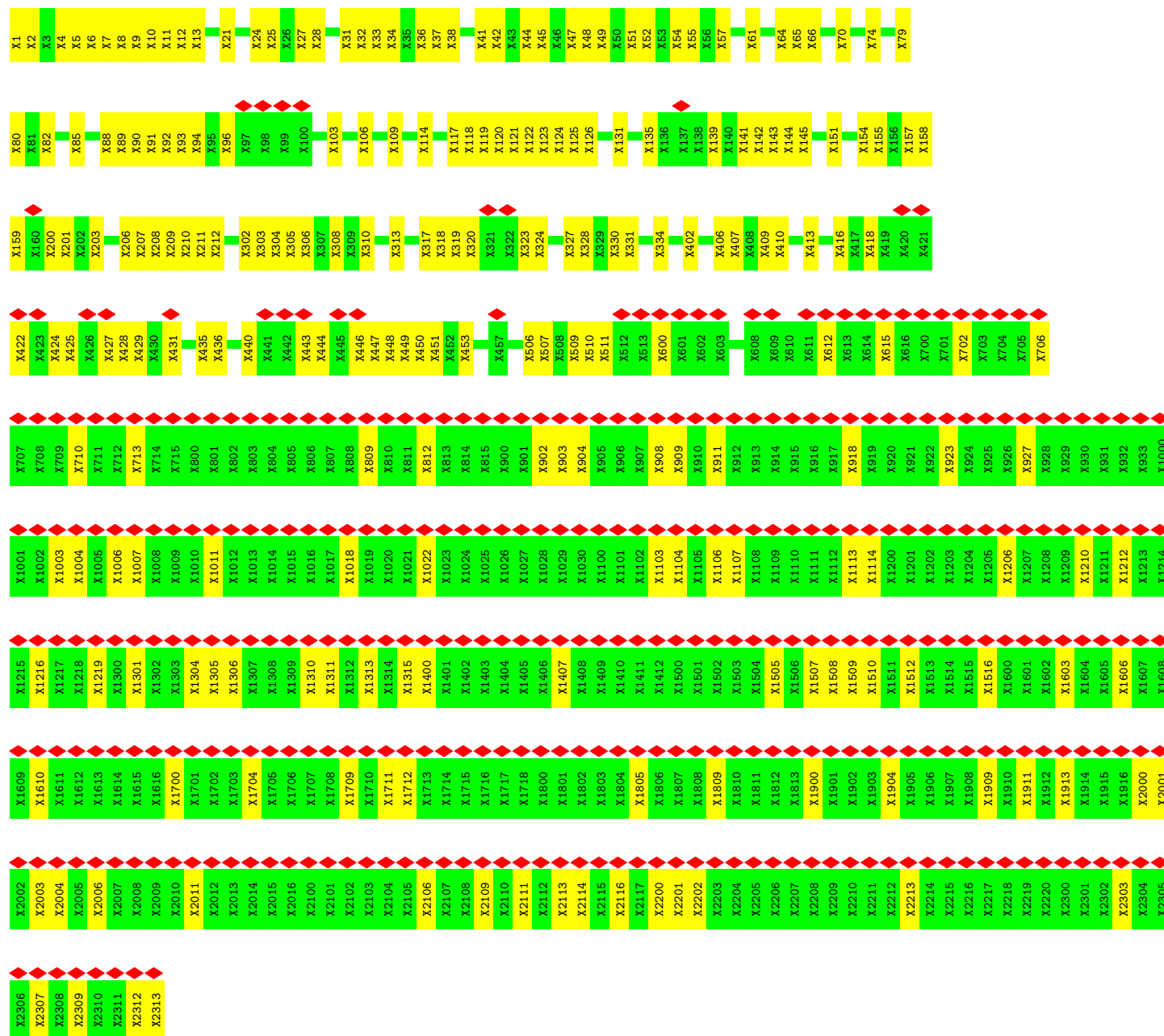
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SERINE/THREONINE-PROTEIN KINASE MTOR



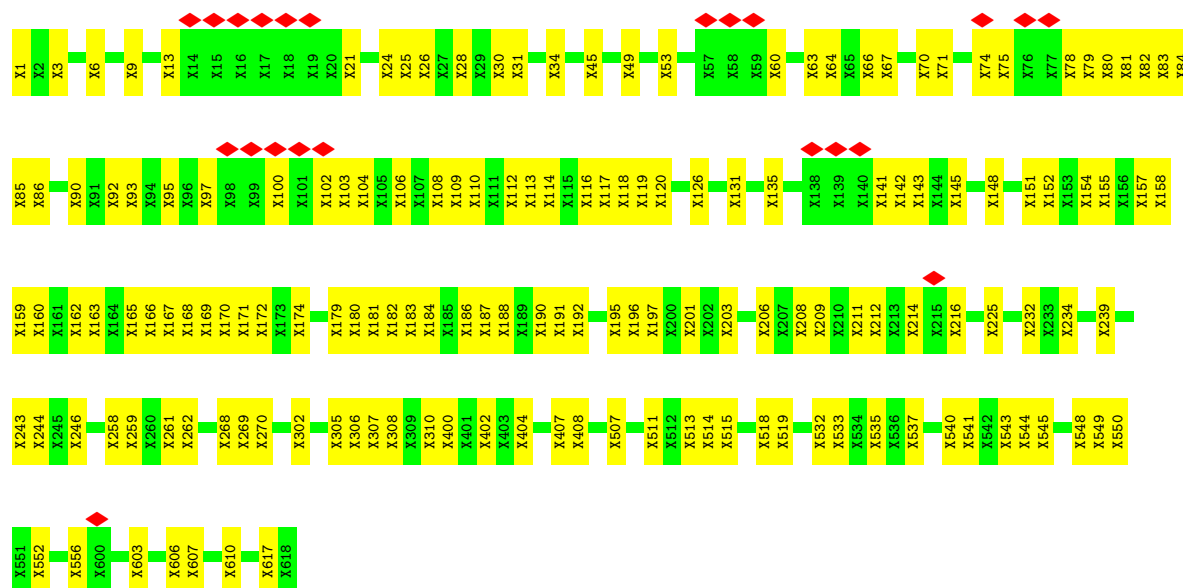


● Molecule 1: SERINE/THREONINE-PROTEIN KINASE MTOR

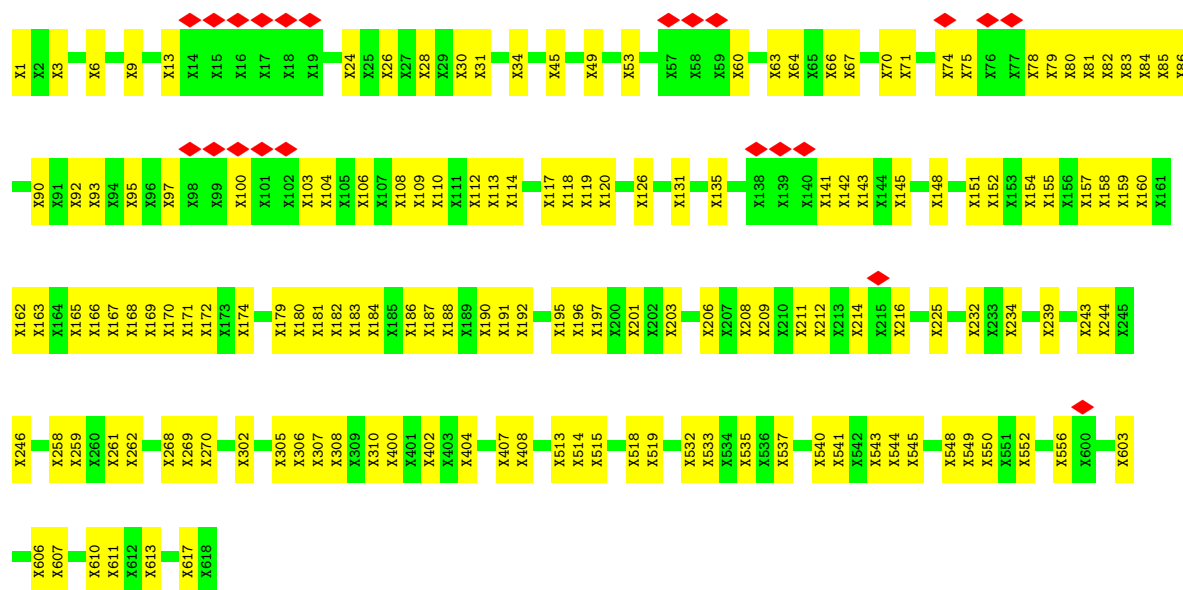


● Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

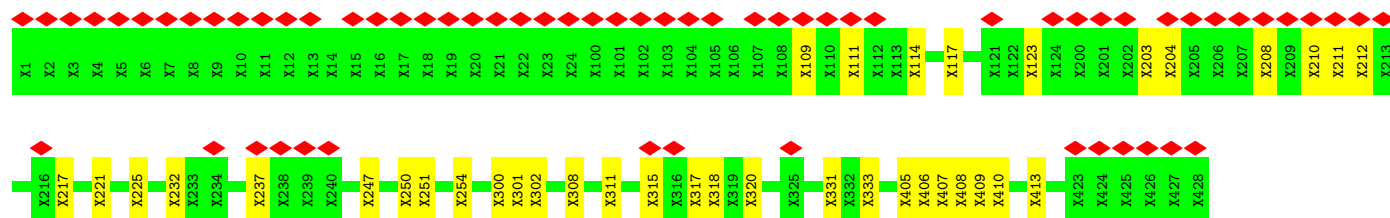
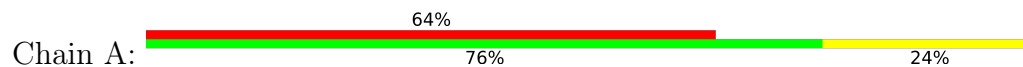


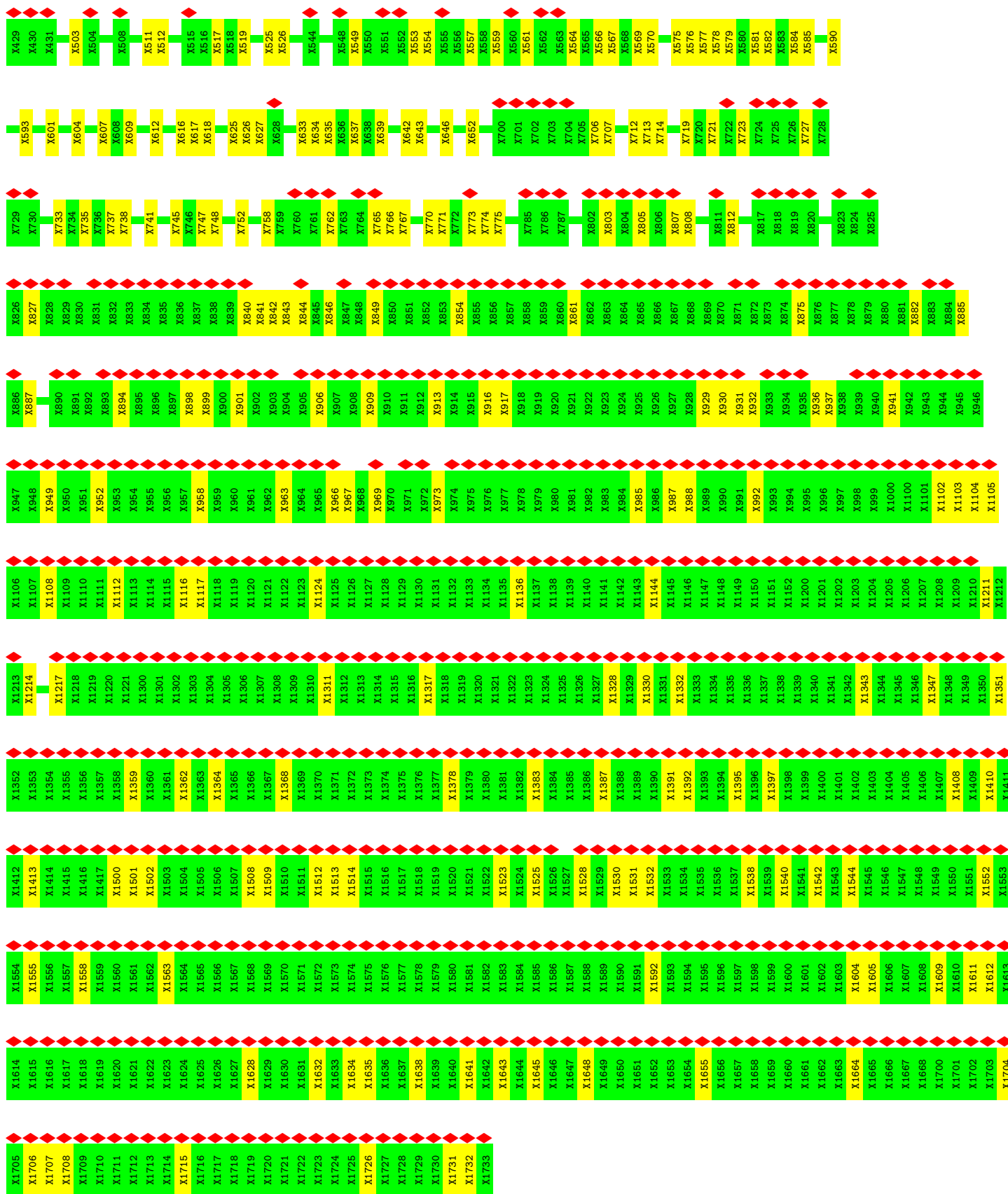


• Molecule 2: SERINE/THREONINE-PROTEIN KINASE MTOR

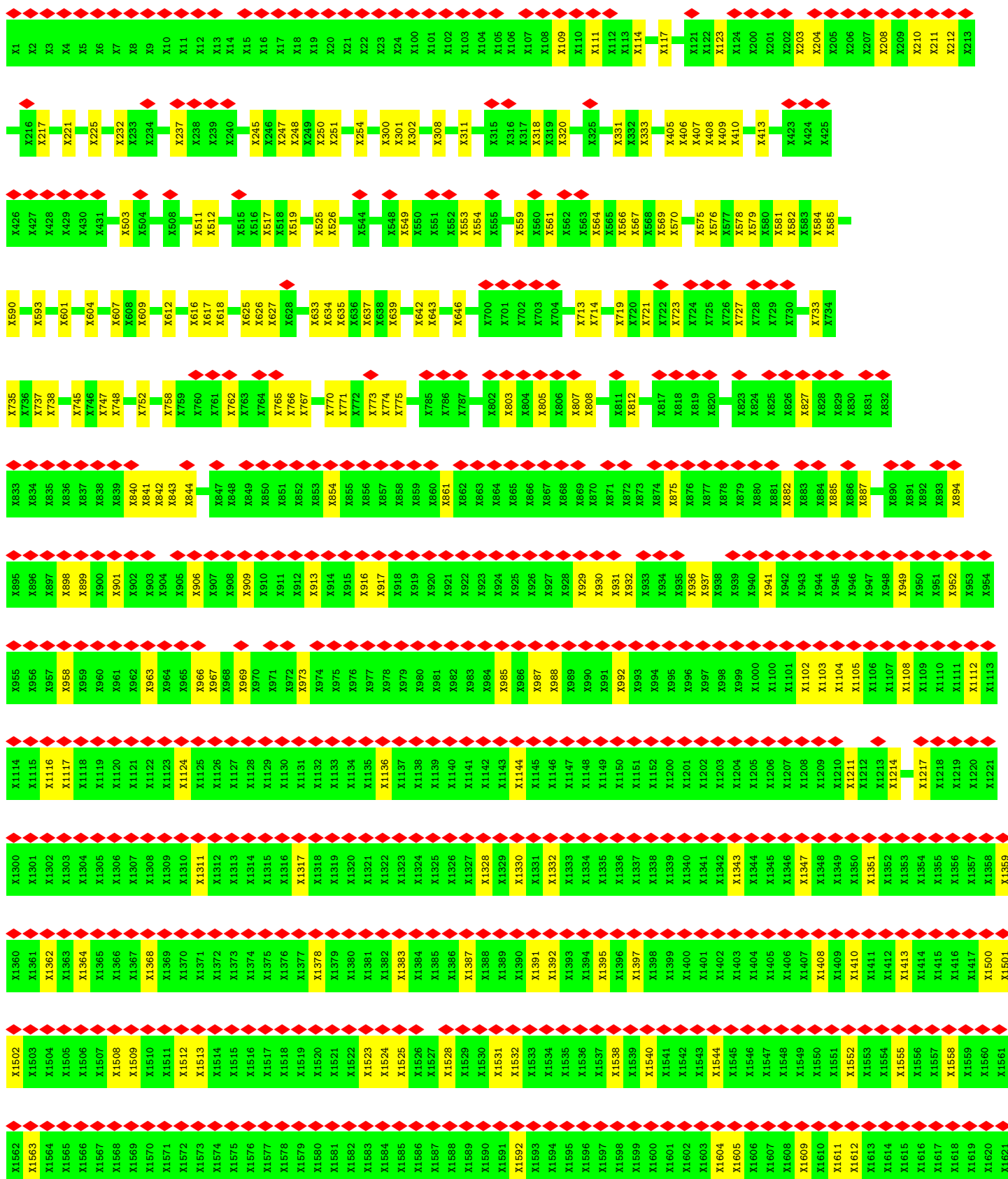
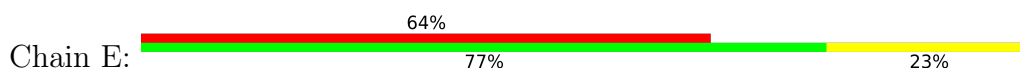


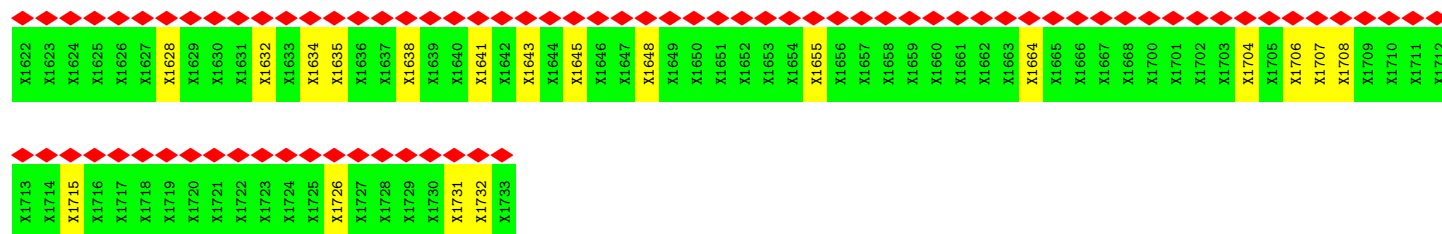
• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR



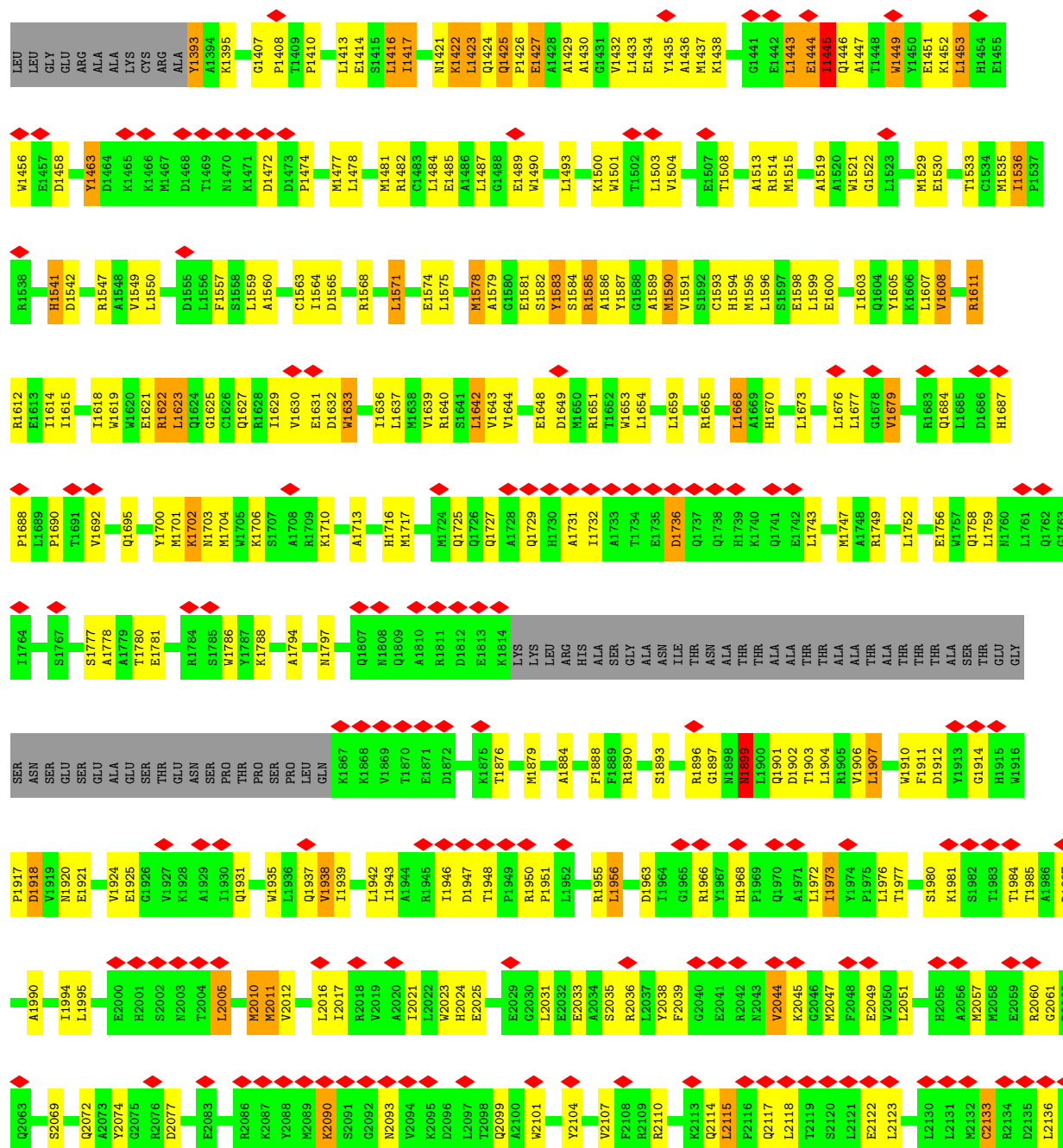


• Molecule 3: REGULATORY-ASSOCIATED PROTEIN OF MTOR



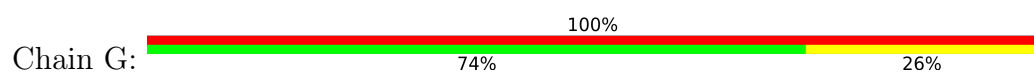


• Molecule 4: SERINE/THREONINE-PROTEIN KINASE MTOR

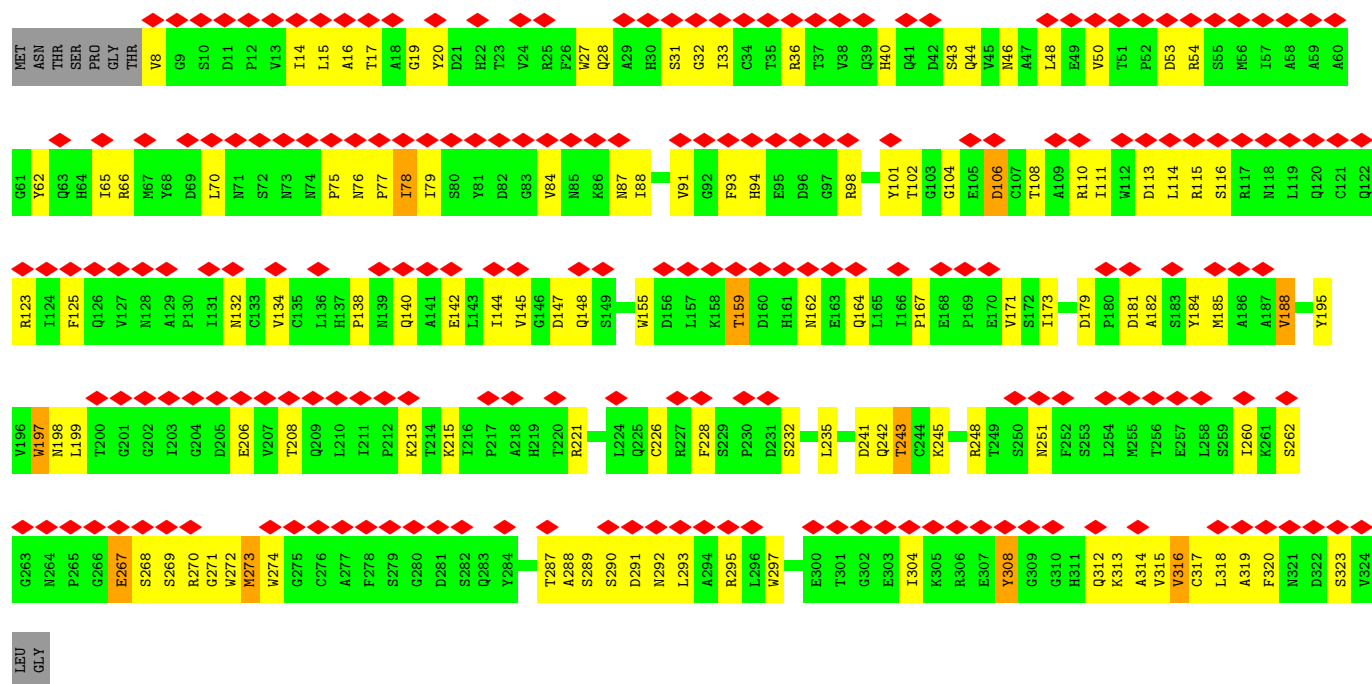




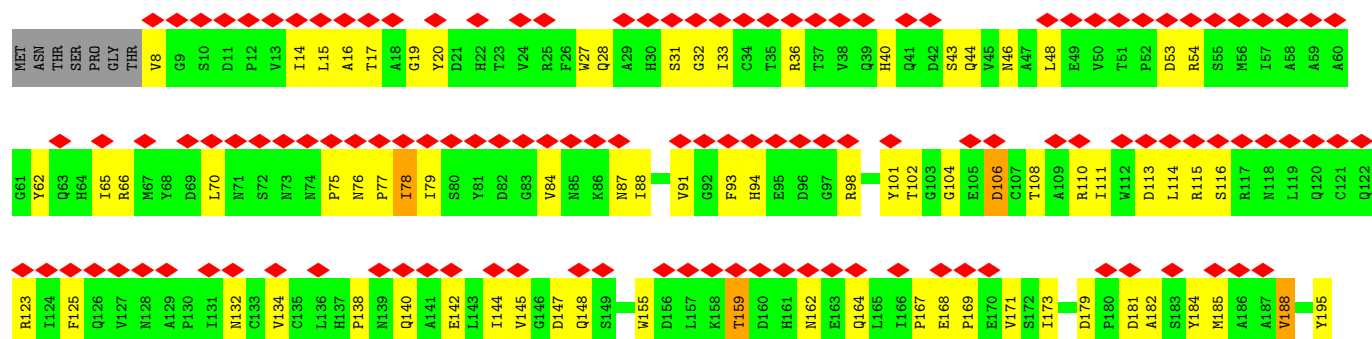


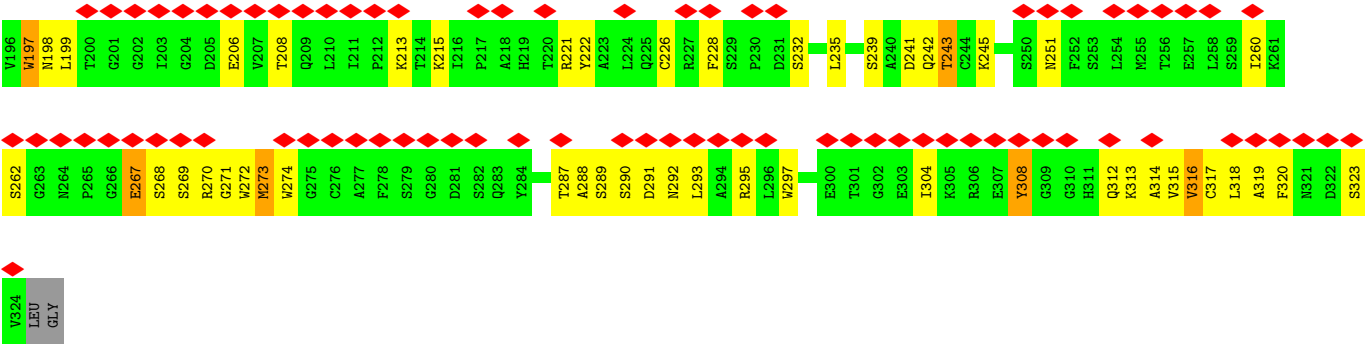


• Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8



• Molecule 6: TARGET OF RAPAMYCIN COMPLEX SUBUNIT LST8





## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, C2               | Depositor |
| Number of particles used             | 309792                  | Depositor |
| Resolution determination method      | Not provided            |           |
| CTF correction method                | EACH IMAGE              | Depositor |
| Microscope                           | FEI TITAN KRIOS         | Depositor |
| Voltage (kV)                         | 300                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                      | Depositor |
| Minimum defocus (nm)                 | 1900                    | Depositor |
| Maximum defocus (nm)                 | 4000                    | Depositor |
| Magnification                        | 100719                  | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value                    | 0.204                   | Depositor |
| Minimum map value                    | -0.046                  | Depositor |
| Average map value                    | 0.001                   | Depositor |
| Map value standard deviation         | 0.010                   | Depositor |
| Recommended contour level            | 0.066                   | Depositor |
| Map size ( $\text{\AA}$ )            | 355.84, 355.84, 355.84  | wwPDB     |
| Map dimensions                       | 256, 256, 256           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.39, 1.39, 1.39        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RAP

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        | $\# Z  > 5$     |
| 4   | B     | 0.46         | 0/8753      | 0.93        | 20/11852 (0.2%) |
| 4   | F     | 0.46         | 0/8753      | 0.92        | 23/11852 (0.2%) |
| 6   | D     | 0.39         | 0/2514      | 0.84        | 0/3426          |
| 6   | H     | 0.39         | 0/2514      | 0.84        | 0/3426          |
| All | All   | 0.45         | 0/22534     | 0.91        | 43/30556 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | 2     | 0                   | 1                   |
| 2   | 4     | 0                   | 1                   |
| 4   | B     | 0                   | 5                   |
| 4   | F     | 0                   | 4                   |
| 6   | D     | 0                   | 1                   |
| 6   | H     | 0                   | 1                   |
| All | All   | 0                   | 13                  |

There are no bond length outliers.

All (43) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 4   | B     | 2115 | LEU  | CA-C-N | -12.40 | 109.13      | 121.65   |
| 4   | B     | 2115 | LEU  | C-N-CA | -12.40 | 109.13      | 121.65   |
| 4   | F     | 2115 | LEU  | CA-C-N | -12.36 | 109.17      | 121.65   |
| 4   | F     | 2115 | LEU  | C-N-CA | -12.36 | 109.17      | 121.65   |
| 4   | F     | 1583 | TYR  | N-CA-C | -10.47 | 100.54      | 113.20   |
| 4   | B     | 1583 | TYR  | N-CA-C | -9.86  | 100.94      | 113.16   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 1445 | ILE  | N-CA-C   | -8.50 | 97.18       | 108.06   |
| 4   | B     | 2375 | ILE  | N-CA-C   | 7.12  | 115.65      | 107.89   |
| 4   | F     | 2375 | ILE  | N-CA-C   | 7.12  | 115.65      | 107.89   |
| 4   | F     | 1914 | GLY  | N-CA-C   | 7.05  | 122.22      | 114.40   |
| 4   | B     | 1623 | LEU  | N-CA-C   | -6.91 | 103.37      | 111.03   |
| 4   | F     | 1583 | TYR  | CA-CB-CG | 6.84  | 126.21      | 113.90   |
| 4   | F     | 1590 | MET  | N-CA-C   | -6.79 | 103.90      | 111.71   |
| 4   | F     | 1623 | LEU  | N-CA-C   | -6.77 | 103.51      | 111.03   |
| 4   | B     | 1590 | MET  | N-CA-C   | -6.74 | 103.96      | 111.71   |
| 4   | B     | 1583 | TYR  | CA-CB-CG | 6.68  | 125.93      | 113.90   |
| 4   | B     | 1914 | GLY  | N-CA-C   | 6.59  | 122.43      | 113.99   |
| 4   | F     | 1968 | HIS  | CA-C-N   | 5.73  | 125.35      | 119.56   |
| 4   | F     | 1968 | HIS  | C-N-CA   | 5.73  | 125.35      | 119.56   |
| 4   | B     | 1968 | HIS  | CA-C-N   | 5.73  | 125.35      | 119.56   |
| 4   | B     | 1968 | HIS  | C-N-CA   | 5.73  | 125.35      | 119.56   |
| 4   | F     | 2168 | ARG  | CA-C-N   | 5.64  | 125.84      | 120.31   |
| 4   | F     | 2168 | ARG  | C-N-CA   | 5.64  | 125.84      | 120.31   |
| 4   | B     | 2168 | ARG  | CA-C-N   | 5.64  | 125.84      | 120.31   |
| 4   | B     | 2168 | ARG  | C-N-CA   | 5.64  | 125.84      | 120.31   |
| 4   | B     | 1443 | LEU  | CB-CA-C  | -5.47 | 109.79      | 117.23   |
| 4   | B     | 2235 | GLY  | N-CA-C   | 5.47  | 118.56      | 110.63   |
| 4   | F     | 1763 | GLY  | N-CA-C   | -5.45 | 106.48      | 112.04   |
| 4   | F     | 2235 | GLY  | N-CA-C   | 5.38  | 118.43      | 110.63   |
| 4   | B     | 1948 | THR  | CA-C-N   | 5.32  | 124.96      | 119.05   |
| 4   | B     | 1948 | THR  | C-N-CA   | 5.32  | 124.96      | 119.05   |
| 4   | F     | 1948 | THR  | CA-C-N   | 5.26  | 124.89      | 119.05   |
| 4   | F     | 1948 | THR  | C-N-CA   | 5.26  | 124.89      | 119.05   |
| 4   | B     | 1423 | LEU  | N-CA-C   | -5.22 | 106.59      | 113.17   |
| 4   | F     | 2157 | ALA  | CA-C-N   | 5.21  | 124.66      | 119.24   |
| 4   | F     | 2157 | ALA  | C-N-CA   | 5.21  | 124.66      | 119.24   |
| 4   | F     | 2212 | ASP  | CA-C-N   | 5.18  | 124.98      | 119.28   |
| 4   | F     | 2212 | ASP  | C-N-CA   | 5.18  | 124.98      | 119.28   |
| 4   | B     | 2212 | ASP  | CA-C-N   | 5.06  | 124.85      | 119.28   |
| 4   | B     | 2212 | ASP  | C-N-CA   | 5.06  | 124.85      | 119.28   |
| 4   | F     | 1950 | ARG  | CA-C-N   | 5.04  | 124.64      | 119.05   |
| 4   | F     | 1950 | ARG  | C-N-CA   | 5.04  | 124.64      | 119.05   |
| 4   | F     | 1443 | LEU  | CB-CA-C  | -5.01 | 110.42      | 117.23   |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | 2     | 216  | UNK  | Peptide |
| 2   | 4     | 216  | UNK  | Peptide |
| 4   | B     | 1444 | GLU  | Peptide |
| 4   | B     | 1445 | ILE  | Peptide |
| 4   | B     | 1649 | ASP  | Peptide |
| 4   | B     | 1897 | GLY  | Peptide |
| 4   | B     | 1899 | ASN  | Peptide |
| 6   | D     | 267  | GLU  | Peptide |
| 4   | F     | 1444 | GLU  | Peptide |
| 4   | F     | 1649 | ASP  | Peptide |
| 4   | F     | 1897 | GLY  | Peptide |
| 4   | F     | 1899 | ASN  | Peptide |
| 6   | H     | 267  | GLU  | 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   | 1     | 3690  | 0        | 3759     | 178     | 0            |
| 1   | 3     | 3690  | 0        | 3760     | 177     | 0            |
| 2   | 2     | 2190  | 0        | 2212     | 115     | 0            |
| 2   | 4     | 2190  | 0        | 2212     | 111     | 0            |
| 3   | A     | 6174  | 0        | 6228     | 150     | 0            |
| 3   | E     | 6174  | 0        | 6228     | 141     | 0            |
| 4   | B     | 8551  | 0        | 8530     | 321     | 0            |
| 4   | F     | 8551  | 0        | 8530     | 324     | 0            |
| 5   | C     | 642   | 0        | 649      | 16      | 0            |
| 5   | G     | 642   | 0        | 648      | 16      | 0            |
| 6   | D     | 2456  | 0        | 2341     | 74      | 0            |
| 6   | H     | 2456  | 0        | 2341     | 73      | 0            |
| 7   | C     | 65    | 0        | 79       | 6       | 0            |
| 7   | G     | 65    | 0        | 79       | 4       | 0            |
| All | All   | 47536 | 0        | 47596    | 1641    | 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 17.

All (1641) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:2419:GLU:HG2 | 4:B:2501:ILE:HG12 | 1.40                     | 1.03              |
| 4:F:2419:GLU:HG2 | 4:F:2501:ILE:HG12 | 1.39                     | 1.02              |
| 1:1:51:UNK:O     | 1:1:55:UNK:N      | 2.06                     | 0.89              |
| 1:3:51:UNK:O     | 1:3:55:UNK:N      | 2.06                     | 0.88              |
| 1:3:41:UNK:HB1   | 1:3:79:UNK:HG1    | 1.58                     | 0.86              |
| 1:1:41:UNK:HB1   | 1:1:79:UNK:HG1    | 1.58                     | 0.83              |
| 4:F:1619:TRP:HA  | 4:F:1622:ARG:HH12 | 1.46                     | 0.81              |
| 1:3:201:UNK:HA   | 1:3:203:UNK:HG3   | 1.62                     | 0.81              |
| 4:B:1595:MET:HG2 | 4:B:1639:VAL:HG21 | 1.62                     | 0.81              |
| 3:E:771:UNK:HA   | 3:E:775:UNK:HB2   | 1.62                     | 0.81              |
| 1:1:2:UNK:H2     | 4:F:1622:ARG:HE   | 1.29                     | 0.80              |
| 5:G:10:UNK:HB1   | 5:G:70:UNK:HB1    | 1.64                     | 0.80              |
| 4:B:1619:TRP:HA  | 4:B:1622:ARG:HH12 | 1.45                     | 0.80              |
| 1:1:201:UNK:HA   | 1:1:203:UNK:HG3   | 1.64                     | 0.80              |
| 3:A:771:UNK:HA   | 3:A:775:UNK:HB2   | 1.63                     | 0.80              |
| 1:1:47:UNK:O     | 1:1:51:UNK:HB1    | 1.82                     | 0.80              |
| 3:A:841:UNK:HB1  | 3:A:844:UNK:HB2   | 1.64                     | 0.79              |
| 1:3:1219:UNK:HG1 | 1:3:1301:UNK:HB2  | 1.65                     | 0.79              |
| 5:C:10:UNK:HB1   | 5:C:70:UNK:HB1    | 1.64                     | 0.79              |
| 1:1:52:UNK:HA    | 1:1:55:UNK:HG3    | 1.65                     | 0.79              |
| 1:3:212:UNK:HA   | 1:3:303:UNK:HB2   | 1.65                     | 0.79              |
| 4:F:2168:ARG:O   | 4:F:2170:ARG:NH1  | 2.16                     | 0.79              |
| 4:F:1595:MET:HG2 | 4:F:1639:VAL:HG21 | 1.62                     | 0.79              |
| 1:3:47:UNK:O     | 1:3:51:UNK:HB1    | 1.82                     | 0.78              |
| 1:3:2:UNK:H2     | 4:B:1622:ARG:HE   | 1.29                     | 0.78              |
| 4:B:2168:ARG:O   | 4:B:2170:ARG:NH1  | 2.16                     | 0.78              |
| 3:E:841:UNK:HB1  | 3:E:844:UNK:HB2   | 1.65                     | 0.78              |
| 2:2:244:UNK:HG1  | 2:2:402:UNK:HB1   | 1.66                     | 0.78              |
| 1:1:212:UNK:HA   | 1:1:303:UNK:HB2   | 1.65                     | 0.77              |
| 1:3:52:UNK:HA    | 1:3:55:UNK:HG3    | 1.66                     | 0.77              |
| 1:1:1219:UNK:HG1 | 1:1:1301:UNK:HB2  | 1.64                     | 0.77              |
| 1:1:90:UNK:HA    | 1:1:93:UNK:HB1    | 1.67                     | 0.77              |
| 1:3:2114:UNK:HG1 | 1:3:2313:UNK:HA   | 1.67                     | 0.77              |
| 4:F:1633:TRP:HA  | 4:F:1636:ILE:HB   | 1.67                     | 0.77              |
| 1:3:1516:UNK:HG1 | 1:3:1603:UNK:HB2  | 1.67                     | 0.76              |
| 4:B:1633:TRP:HA  | 4:B:1636:ILE:HB   | 1.67                     | 0.76              |
| 1:3:90:UNK:HA    | 1:3:93:UNK:HB1    | 1.67                     | 0.76              |
| 2:4:244:UNK:HG1  | 2:4:402:UNK:HB1   | 1.67                     | 0.76              |
| 3:A:582:UNK:HG3  | 3:A:635:UNK:HG1   | 1.68                     | 0.76              |
| 1:1:1516:UNK:HG1 | 1:1:1603:UNK:HB2  | 1.67                     | 0.76              |
| 1:3:118:UNK:O    | 1:3:120:UNK:N     | 2.19                     | 0.76              |
| 3:E:584:UNK:HB1  | 3:E:737:UNK:HG1   | 1.69                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:320:UNK:O    | 1:1:324:UNK:N     | 2.20                     | 0.75              |
| 1:3:320:UNK:O    | 1:3:324:UNK:N     | 2.20                     | 0.75              |
| 3:E:582:UNK:HG3  | 3:E:635:UNK:HG1   | 1.66                     | 0.75              |
| 1:1:118:UNK:O    | 1:1:120:UNK:N     | 2.19                     | 0.75              |
| 1:1:2114:UNK:HG1 | 1:1:2313:UNK:HA   | 1.67                     | 0.74              |
| 2:4:552:UNK:HG1  | 4:F:2304:TRP:HZ2  | 1.51                     | 0.74              |
| 3:E:1413:UNK:HB1 | 3:E:1513:UNK:HG1  | 1.69                     | 0.74              |
| 4:F:2302:LEU:O   | 4:F:2306:LYS:N    | 2.20                     | 0.74              |
| 1:1:154:UNK:HG3  | 3:A:643:UNK:HB1   | 1.67                     | 0.74              |
| 1:3:131:UNK:HB1  | 1:3:144:UNK:HG1   | 1.69                     | 0.74              |
| 4:B:2302:LEU:O   | 4:B:2306:LYS:N    | 2.20                     | 0.74              |
| 1:3:154:UNK:HG3  | 3:E:643:UNK:HB1   | 1.67                     | 0.74              |
| 3:A:1634:UNK:HG1 | 3:A:1704:UNK:HA   | 1.70                     | 0.74              |
| 3:A:584:UNK:HB1  | 3:A:737:UNK:HG1   | 1.69                     | 0.73              |
| 2:2:552:UNK:HG1  | 4:B:2304:TRP:HZ2  | 1.53                     | 0.73              |
| 3:A:1413:UNK:HB1 | 3:A:1513:UNK:HG1  | 1.69                     | 0.73              |
| 4:F:2260:LEU:HB3 | 4:F:2263:ILE:HB   | 1.70                     | 0.73              |
| 1:1:305:UNK:HB2  | 2:2:75:UNK:HG1    | 1.69                     | 0.73              |
| 3:E:1634:UNK:HG1 | 3:E:1704:UNK:HA   | 1.71                     | 0.73              |
| 1:1:131:UNK:HB1  | 1:1:144:UNK:HG1   | 1.70                     | 0.73              |
| 2:4:53:UNK:HA    | 2:4:95:UNK:HG1    | 1.70                     | 0.73              |
| 4:F:2163:ILE:HB  | 4:F:2169:PRO:HG2  | 1.71                     | 0.72              |
| 2:2:53:UNK:HA    | 2:2:95:UNK:HG1    | 1.70                     | 0.72              |
| 3:E:1112:UNK:HB1 | 3:E:1124:UNK:HG1  | 1.71                     | 0.72              |
| 1:3:911:UNK:HG3  | 1:3:918:UNK:HA    | 1.70                     | 0.72              |
| 3:A:1112:UNK:HB1 | 3:A:1124:UNK:HG1  | 1.71                     | 0.72              |
| 1:3:1:UNK:HG1    | 4:B:1598:GLU:HG2  | 1.71                     | 0.72              |
| 4:B:2260:LEU:HB3 | 4:B:2263:ILE:HB   | 1.69                     | 0.72              |
| 6:H:288:ALA:HB2  | 6:H:318:LEU:HG    | 1.72                     | 0.72              |
| 2:2:603:UNK:HA   | 2:2:606:UNK:HB1   | 1.72                     | 0.72              |
| 6:D:288:ALA:HB2  | 6:D:318:LEU:HG    | 1.72                     | 0.72              |
| 1:3:305:UNK:HB2  | 2:4:75:UNK:HG1    | 1.69                     | 0.71              |
| 4:B:2404:MET:HG3 | 4:B:2521:VAL:HG22 | 1.73                     | 0.71              |
| 4:F:2404:MET:HG3 | 4:F:2521:VAL:HG22 | 1.73                     | 0.71              |
| 1:1:911:UNK:HG3  | 1:1:918:UNK:HA    | 1.71                     | 0.71              |
| 4:B:2415:MET:SD  | 4:B:2505:ARG:NH1  | 2.63                     | 0.71              |
| 4:F:2300:ALA:HB2 | 4:F:2386:ALA:HA   | 1.71                     | 0.71              |
| 4:F:2415:MET:SD  | 4:F:2505:ARG:NH1  | 2.64                     | 0.71              |
| 1:1:1:UNK:HG1    | 4:F:1598:GLU:HG2  | 1.71                     | 0.71              |
| 2:2:31:UNK:HA    | 2:2:34:UNK:HB1    | 1.73                     | 0.70              |
| 4:B:2300:ALA:HB2 | 4:B:2386:ALA:HA   | 1.71                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:1393:TYR:HB2  | 4:F:1423:LEU:HD22 | 1.74                     | 0.70              |
| 4:B:1393:TYR:HB2  | 4:B:1423:LEU:HD22 | 1.74                     | 0.70              |
| 1:1:38:UNK:HG1    | 4:F:1618:ILE:HG22 | 1.74                     | 0.69              |
| 1:3:38:UNK:HG1    | 4:B:1618:ILE:HG22 | 1.74                     | 0.69              |
| 2:4:603:UNK:HA    | 2:4:606:UNK:HB1   | 1.72                     | 0.69              |
| 4:B:2332:TYR:O    | 4:B:2507:LYS:NZ   | 2.22                     | 0.69              |
| 4:F:2332:TYR:O    | 4:F:2507:LYS:NZ   | 2.22                     | 0.69              |
| 3:E:410:UNK:O     | 3:E:413:UNK:N     | 2.26                     | 0.69              |
| 1:3:155:UNK:O     | 1:3:157:UNK:N     | 2.26                     | 0.69              |
| 3:E:721:UNK:HB1   | 3:E:733:UNK:HB1   | 1.74                     | 0.69              |
| 4:F:1493:LEU:HD23 | 4:F:1519:ALA:HB2  | 1.75                     | 0.69              |
| 4:F:2222:ILE:HG12 | 4:F:2327:MET:HG2  | 1.75                     | 0.69              |
| 6:D:32:GLY:HA2    | 6:D:308:TYR:HD2   | 1.58                     | 0.69              |
| 1:1:158:UNK:HA    | 3:A:713:UNK:HG1   | 1.75                     | 0.69              |
| 1:3:2111:UNK:HG2  | 1:3:2312:UNK:HG1  | 1.75                     | 0.69              |
| 3:E:887:UNK:HA    | 3:E:930:UNK:HG1   | 1.76                     | 0.68              |
| 4:F:2339:ARG:NH2  | 4:F:2356:ILE:O    | 2.26                     | 0.68              |
| 4:B:2222:ILE:HG12 | 4:B:2327:MET:HG2  | 1.75                     | 0.68              |
| 3:E:203:UNK:HB1   | 3:E:208:UNK:HG1   | 1.76                     | 0.68              |
| 3:A:203:UNK:HB1   | 3:A:208:UNK:HG1   | 1.75                     | 0.68              |
| 3:A:251:UNK:HA    | 3:A:254:UNK:HB1   | 1.75                     | 0.68              |
| 3:A:721:UNK:HB1   | 3:A:733:UNK:HB1   | 1.74                     | 0.68              |
| 2:4:31:UNK:HA     | 2:4:34:UNK:HB1    | 1.74                     | 0.68              |
| 4:B:2339:ARG:NH2  | 4:B:2356:ILE:O    | 2.26                     | 0.68              |
| 1:1:2111:UNK:HG2  | 1:1:2312:UNK:HG1  | 1.75                     | 0.68              |
| 2:2:92:UNK:HB1    | 2:2:100:UNK:HG1   | 1.76                     | 0.68              |
| 1:1:51:UNK:HG2    | 1:1:55:UNK:HB1    | 1.76                     | 0.68              |
| 1:3:51:UNK:HG2    | 1:3:55:UNK:HB1    | 1.76                     | 0.68              |
| 2:4:92:UNK:HB1    | 2:4:100:UNK:HG1   | 1.75                     | 0.68              |
| 3:A:410:UNK:O     | 3:A:413:UNK:N     | 2.25                     | 0.68              |
| 6:H:32:GLY:HA2    | 6:H:308:TYR:HD2   | 1.58                     | 0.68              |
| 4:B:2077:ASP:OD2  | 4:B:2110:ARG:NH2  | 2.27                     | 0.68              |
| 4:B:2163:ILE:HB   | 4:B:2169:PRO:HG2  | 1.74                     | 0.68              |
| 1:3:1505:UNK:HA   | 1:3:1508:UNK:HB1  | 1.75                     | 0.68              |
| 1:1:155:UNK:O     | 1:1:157:UNK:N     | 2.26                     | 0.67              |
| 4:F:2077:ASP:OD2  | 4:F:2110:ARG:NH2  | 2.27                     | 0.67              |
| 1:3:158:UNK:HA    | 3:E:713:UNK:HG1   | 1.75                     | 0.67              |
| 6:D:91:VAL:HG12   | 6:D:102:THR:HG22  | 1.77                     | 0.67              |
| 2:4:118:UNK:HG2   | 2:4:158:UNK:HA    | 1.76                     | 0.67              |
| 4:F:2337:GLY:O    | 4:F:2339:ARG:NH1  | 2.28                     | 0.67              |
| 3:E:406:UNK:HG1   | 3:E:525:UNK:HG2   | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:887:UNK:HA    | 3:A:930:UNK:HG1   | 1.75                     | 0.67              |
| 1:1:1505:UNK:HA   | 1:1:1508:UNK:HB1  | 1.75                     | 0.67              |
| 2:2:66:UNK:O      | 2:2:70:UNK:N      | 2.28                     | 0.67              |
| 1:3:122:UNK:HA    | 1:3:125:UNK:HB1   | 1.76                     | 0.67              |
| 1:3:157:UNK:HG2   | 1:3:158:UNK:HG3   | 1.76                     | 0.67              |
| 4:B:2395:ASN:O    | 4:B:2399:THR:OG1  | 2.10                     | 0.67              |
| 3:A:406:UNK:HG1   | 3:A:525:UNK:HG2   | 1.77                     | 0.66              |
| 4:B:1493:LEU:HD23 | 4:B:1519:ALA:HB2  | 1.75                     | 0.66              |
| 1:1:157:UNK:HG2   | 1:1:158:UNK:HG3   | 1.76                     | 0.66              |
| 4:B:2337:GLY:O    | 4:B:2339:ARG:NH1  | 2.28                     | 0.66              |
| 1:3:904:UNK:HG1   | 1:3:1003:UNK:HG3  | 1.78                     | 0.66              |
| 4:B:2247:HIS:HB2  | 4:B:2341:PRO:HB2  | 1.78                     | 0.66              |
| 3:E:251:UNK:HA    | 3:E:254:UNK:HB1   | 1.76                     | 0.66              |
| 4:F:1690:PRO:HB2  | 4:F:1692:VAL:HG22 | 1.78                     | 0.66              |
| 6:H:91:VAL:HG12   | 6:H:102:THR:HG22  | 1.77                     | 0.66              |
| 1:1:122:UNK:HA    | 1:1:125:UNK:HB1   | 1.76                     | 0.66              |
| 1:3:122:UNK:O     | 1:3:126:UNK:N     | 2.29                     | 0.66              |
| 4:F:2506:ASP:HA   | 4:F:2511:ARG:HB2  | 1.78                     | 0.66              |
| 4:F:2247:HIS:HB2  | 4:F:2341:PRO:HB2  | 1.76                     | 0.66              |
| 4:F:1963:ASP:OD1  | 4:F:1966:ARG:NH2  | 2.29                     | 0.66              |
| 2:2:118:UNK:HG2   | 2:2:158:UNK:HA    | 1.77                     | 0.66              |
| 1:1:122:UNK:O     | 1:1:126:UNK:N     | 2.29                     | 0.65              |
| 4:B:1963:ASP:OD1  | 4:B:1966:ARG:NH2  | 2.29                     | 0.65              |
| 4:B:2319:ASN:O    | 4:B:2323:SER:OG   | 2.14                     | 0.65              |
| 4:B:1586:ALA:O    | 4:B:1590:MET:HB2  | 1.96                     | 0.65              |
| 4:F:1578:MET:SD   | 4:F:1579:ALA:N    | 2.60                     | 0.65              |
| 1:1:6:UNK:O       | 1:1:10:UNK:N      | 2.29                     | 0.65              |
| 1:1:904:UNK:HG1   | 1:1:1003:UNK:HG3  | 1.77                     | 0.65              |
| 2:4:145:UNK:HA    | 2:4:148:UNK:HB2   | 1.77                     | 0.65              |
| 5:G:29:UNK:HB1    | 5:G:35:UNK:HA     | 1.78                     | 0.65              |
| 1:3:1106:UNK:HG1  | 1:3:1305:UNK:HG3  | 1.78                     | 0.65              |
| 4:F:1586:ALA:O    | 4:F:1590:MET:HB2  | 1.96                     | 0.65              |
| 4:F:2161:GLN:O    | 4:F:2171:LYS:N    | 2.25                     | 0.65              |
| 1:3:6:UNK:O       | 1:3:10:UNK:N      | 2.29                     | 0.65              |
| 5:C:29:UNK:HB1    | 5:C:35:UNK:HA     | 1.79                     | 0.65              |
| 3:E:1211:UNK:HA   | 3:E:1214:UNK:HB2  | 1.79                     | 0.65              |
| 4:F:2240:VAL:HG21 | 4:F:2354:LEU:HD22 | 1.77                     | 0.65              |
| 2:4:66:UNK:O      | 2:4:70:UNK:N      | 2.29                     | 0.65              |
| 4:B:2408:ARG:NH2  | 4:B:2519:LEU:O    | 2.30                     | 0.65              |
| 4:B:2506:ASP:HA   | 4:B:2511:ARG:HB2  | 1.79                     | 0.65              |
| 4:F:1622:ARG:HA   | 4:F:1625:GLY:HA3  | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:48:UNK:O      | 1:1:52:UNK:HB1    | 1.97                     | 0.65              |
| 1:1:310:UNK:HA    | 1:1:313:UNK:HB1   | 1.79                     | 0.65              |
| 1:3:48:UNK:O      | 1:3:52:UNK:HB1    | 1.96                     | 0.65              |
| 3:E:549:UNK:HG3   | 3:E:553:UNK:HB1   | 1.79                     | 0.65              |
| 4:F:2319:ASN:O    | 4:F:2323:SER:OG   | 2.15                     | 0.65              |
| 4:B:2240:VAL:HG21 | 4:B:2354:LEU:HD22 | 1.77                     | 0.64              |
| 2:2:145:UNK:HA    | 2:2:148:UNK:HB2   | 1.77                     | 0.64              |
| 4:B:1622:ARG:HA   | 4:B:1625:GLY:HA3  | 1.79                     | 0.64              |
| 4:B:1896:ARG:HH21 | 4:B:1931:GLN:HG3  | 1.61                     | 0.64              |
| 1:3:310:UNK:HA    | 1:3:313:UNK:HB1   | 1.79                     | 0.64              |
| 1:3:1704:UNK:HG2  | 1:3:1904:UNK:HG1  | 1.79                     | 0.64              |
| 4:B:1690:PRO:HB2  | 4:B:1692:VAL:HG22 | 1.78                     | 0.64              |
| 6:D:134:VAL:HG22  | 6:D:145:VAL:HG22  | 1.79                     | 0.64              |
| 4:F:1896:ARG:HH21 | 4:F:1931:GLN:HG3  | 1.61                     | 0.64              |
| 2:4:183:UNK:HA    | 2:4:186:UNK:HB1   | 1.78                     | 0.64              |
| 1:1:331:UNK:HB1   | 1:1:407:UNK:HB1   | 1.80                     | 0.64              |
| 1:3:702:UNK:HG1   | 1:3:812:UNK:HG1   | 1.78                     | 0.64              |
| 3:A:549:UNK:HG3   | 3:A:553:UNK:HB1   | 1.80                     | 0.64              |
| 1:1:1106:UNK:HG1  | 1:1:1305:UNK:HG3  | 1.78                     | 0.64              |
| 2:2:163:UNK:HA    | 2:2:166:UNK:HB2   | 1.80                     | 0.64              |
| 3:E:123:UNK:HA    | 3:E:308:UNK:HB2   | 1.80                     | 0.64              |
| 1:1:1704:UNK:HG2  | 1:1:1904:UNK:HG1  | 1.78                     | 0.63              |
| 4:B:1590:MET:O    | 4:B:1594:HIS:HB2  | 1.98                     | 0.63              |
| 4:B:2178:ASN:H    | 4:B:2178:ASN:HD22 | 1.46                     | 0.63              |
| 3:E:901:UNK:HG3   | 3:E:941:UNK:HG3   | 1.80                     | 0.63              |
| 4:F:1590:MET:O    | 4:F:1594:HIS:HB2  | 1.99                     | 0.63              |
| 1:1:702:UNK:HG1   | 1:1:812:UNK:HG1   | 1.79                     | 0.63              |
| 3:A:1211:UNK:HA   | 3:A:1214:UNK:HB2  | 1.79                     | 0.63              |
| 4:B:2421:PHE:HA   | 4:B:2424:ASP:HB2  | 1.80                     | 0.63              |
| 3:A:901:UNK:HG3   | 3:A:941:UNK:HG3   | 1.80                     | 0.63              |
| 4:F:2408:ARG:NH2  | 4:F:2519:LEU:O    | 2.31                     | 0.63              |
| 6:D:46:ASN:ND2    | 6:D:87:ASN:OD1    | 2.31                     | 0.63              |
| 3:E:1413:UNK:HG3  | 3:E:1523:UNK:HG1  | 1.80                     | 0.63              |
| 3:A:1413:UNK:HG3  | 3:A:1523:UNK:HG1  | 1.80                     | 0.63              |
| 4:B:1749:ARG:HG2  | 4:B:1786:TRP:CH2  | 2.34                     | 0.63              |
| 4:F:2363:GLU:O    | 4:F:2367:THR:OG1  | 2.17                     | 0.63              |
| 4:F:2421:PHE:HA   | 4:F:2424:ASP:HB2  | 1.81                     | 0.63              |
| 2:4:163:UNK:HA    | 2:4:166:UNK:HB2   | 1.79                     | 0.63              |
| 4:F:2395:ASN:O    | 4:F:2399:THR:OG1  | 2.10                     | 0.63              |
| 1:3:331:UNK:HB1   | 1:3:407:UNK:HB1   | 1.80                     | 0.62              |
| 3:A:123:UNK:HA    | 3:A:308:UNK:HB2   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1391:UNK:HG3  | 3:E:1500:UNK:HB1  | 1.80                     | 0.62              |
| 1:1:119:UNK:O     | 1:1:121:UNK:N     | 2.33                     | 0.62              |
| 2:4:80:UNK:HA     | 2:4:120:UNK:HG1   | 1.81                     | 0.62              |
| 2:4:154:UNK:O     | 2:4:158:UNK:HB1   | 1.99                     | 0.62              |
| 3:A:1391:UNK:HG3  | 3:A:1500:UNK:HB1  | 1.80                     | 0.62              |
| 4:B:2363:GLU:O    | 4:B:2367:THR:OG1  | 2.17                     | 0.62              |
| 2:2:154:UNK:O     | 2:2:158:UNK:HB1   | 1.99                     | 0.62              |
| 6:H:46:ASN:ND2    | 6:H:87:ASN:OD1    | 2.31                     | 0.62              |
| 6:H:134:VAL:HG22  | 6:H:145:VAL:HG22  | 1.79                     | 0.62              |
| 3:E:1317:UNK:HG1  | 3:E:1351:UNK:HA   | 1.81                     | 0.62              |
| 4:F:1749:ARG:HG2  | 4:F:1786:TRP:CH2  | 2.34                     | 0.62              |
| 3:A:311:UNK:HG2   | 3:A:320:UNK:HG1   | 1.81                     | 0.62              |
| 6:H:181:ASP:OD2   | 6:H:232:SER:OG    | 2.18                     | 0.62              |
| 1:3:119:UNK:O     | 1:3:121:UNK:N     | 2.33                     | 0.62              |
| 6:D:195:TYR:OH    | 6:D:215:LYS:NZ    | 2.32                     | 0.61              |
| 4:F:2270:ARG:O    | 6:H:313:LYS:NZ    | 2.27                     | 0.61              |
| 4:B:1636:ILE:HG22 | 4:B:1637:LEU:HD23 | 1.81                     | 0.61              |
| 4:B:2161:GLN:O    | 4:B:2171:LYS:N    | 2.25                     | 0.61              |
| 4:F:1581:GLU:CB   | 4:F:1585:ARG:HB2  | 2.30                     | 0.61              |
| 2:4:90:UNK:HG3    | 2:4:131:UNK:HG1   | 1.83                     | 0.61              |
| 6:D:36:ARG:HH12   | 6:D:75:PRO:HD2    | 1.65                     | 0.61              |
| 6:D:106:ASP:OD2   | 6:D:108:THR:OG1   | 2.18                     | 0.61              |
| 3:E:898:UNK:HG3   | 3:E:899:UNK:HG2   | 1.82                     | 0.61              |
| 6:H:36:ARG:HH12   | 6:H:75:PRO:HD2    | 1.64                     | 0.61              |
| 1:3:328:UNK:HB2   | 1:3:431:UNK:HB2   | 1.82                     | 0.61              |
| 4:B:2303:LEU:HA   | 4:B:2306:LYS:HB2  | 1.83                     | 0.61              |
| 1:1:139:UNK:O     | 1:1:141:UNK:N     | 2.33                     | 0.61              |
| 1:1:328:UNK:HB2   | 1:1:431:UNK:HB2   | 1.81                     | 0.61              |
| 4:B:1581:GLU:CB   | 4:B:1585:ARG:HB2  | 2.30                     | 0.61              |
| 4:F:1549:VAL:HG13 | 4:F:1642:LEU:HD11 | 1.82                     | 0.61              |
| 2:4:182:UNK:HG2   | 2:4:183:UNK:HG2   | 1.83                     | 0.61              |
| 3:A:114:UNK:HA    | 3:A:300:UNK:HA    | 1.83                     | 0.61              |
| 3:E:311:UNK:HG2   | 3:E:320:UNK:HG1   | 1.81                     | 0.61              |
| 1:3:511:UNK:HA    | 1:3:600:UNK:HB1   | 1.83                     | 0.61              |
| 2:4:155:UNK:HB1   | 2:4:190:UNK:HG1   | 1.83                     | 0.61              |
| 3:A:898:UNK:HG3   | 3:A:899:UNK:HG2   | 1.82                     | 0.61              |
| 4:B:1786:TRP:CZ2  | 4:B:1788:LYS:HD3  | 2.36                     | 0.61              |
| 4:F:1636:ILE:HG22 | 4:F:1637:LEU:HD23 | 1.80                     | 0.61              |
| 2:2:155:UNK:HB1   | 2:2:190:UNK:HG1   | 1.83                     | 0.61              |
| 2:2:545:UNK:HG3   | 4:B:1395:LYS:HZ3  | 1.66                     | 0.61              |
| 6:H:167:PRO:HG3   | 6:H:197:TRP:HZ2   | 1.66                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:80:UNK:HA     | 2:2:120:UNK:HG1   | 1.81                     | 0.61              |
| 3:A:1317:UNK:HG1  | 3:A:1351:UNK:HA   | 1.82                     | 0.61              |
| 4:B:1578:MET:SD   | 4:B:1579:ALA:N    | 2.60                     | 0.61              |
| 3:E:114:UNK:HA    | 3:E:300:UNK:HA    | 1.83                     | 0.61              |
| 4:F:1490:TRP:CE3  | 4:F:1519:ALA:HA   | 2.35                     | 0.61              |
| 1:3:139:UNK:O     | 1:3:141:UNK:N     | 2.34                     | 0.60              |
| 1:3:203:UNK:O     | 1:3:207:UNK:HB1   | 2.00                     | 0.60              |
| 3:A:117:UNK:HA    | 3:A:301:UNK:HG2   | 1.83                     | 0.60              |
| 3:E:117:UNK:HA    | 3:E:301:UNK:HG2   | 1.83                     | 0.60              |
| 4:B:1549:VAL:HG13 | 4:B:1642:LEU:HD11 | 1.81                     | 0.60              |
| 6:D:167:PRO:HG3   | 6:D:197:TRP:HZ2   | 1.66                     | 0.60              |
| 4:F:2178:ASN:HD22 | 4:F:2178:ASN:H    | 1.47                     | 0.60              |
| 6:H:138:PRO:HG2   | 6:H:182:ALA:HB2   | 1.83                     | 0.60              |
| 2:2:90:UNK:HG3    | 2:2:131:UNK:HG1   | 1.82                     | 0.60              |
| 4:B:1490:TRP:CE3  | 4:B:1519:ALA:HA   | 2.36                     | 0.60              |
| 6:H:195:TYR:OH    | 6:H:215:LYS:NZ    | 2.32                     | 0.60              |
| 4:F:1786:TRP:CZ2  | 4:F:1788:LYS:HD3  | 2.36                     | 0.60              |
| 4:F:2256:LYS:HZ2  | 4:F:2257:LYS:HE3  | 1.65                     | 0.60              |
| 6:H:15:LEU:HD13   | 6:H:320:PHE:HD1   | 1.66                     | 0.60              |
| 1:1:511:UNK:HA    | 1:1:600:UNK:HB1   | 1.83                     | 0.60              |
| 2:4:513:UNK:HG1   | 2:4:550:UNK:HB1   | 1.83                     | 0.60              |
| 3:E:1538:UNK:HG1  | 3:E:1563:UNK:HG1  | 1.84                     | 0.60              |
| 6:D:111:ILE:HB    | 6:D:123:ARG:HB2   | 1.83                     | 0.60              |
| 6:H:111:ILE:HB    | 6:H:123:ARG:HB2   | 1.84                     | 0.60              |
| 1:1:203:UNK:O     | 1:1:207:UNK:HB1   | 2.01                     | 0.60              |
| 1:3:2201:UNK:HG2  | 1:3:2202:UNK:HG3  | 1.84                     | 0.60              |
| 4:B:2141:PRO:HB3  | 4:B:2228:ILE:HG21 | 1.84                     | 0.60              |
| 4:F:2339:ARG:NH2  | 4:F:2343:ASN:OD1  | 2.35                     | 0.60              |
| 2:2:209:UNK:HB2   | 2:2:246:UNK:HB2   | 1.84                     | 0.59              |
| 4:B:1529:MET:O    | 4:B:1533:THR:OG1  | 2.16                     | 0.59              |
| 6:D:15:LEU:HD13   | 6:D:320:PHE:HD1   | 1.67                     | 0.59              |
| 6:H:106:ASP:OD2   | 6:H:108:THR:OG1   | 2.19                     | 0.59              |
| 4:B:2339:ARG:NH2  | 4:B:2343:ASN:OD1  | 2.35                     | 0.59              |
| 4:B:2347:ASP:OD1  | 4:B:2350:SER:N    | 2.35                     | 0.59              |
| 4:F:2303:LEU:HA   | 4:F:2306:LYS:HB2  | 1.83                     | 0.59              |
| 2:2:182:UNK:HG2   | 2:2:183:UNK:HG2   | 1.83                     | 0.59              |
| 4:B:2031:LEU:O    | 4:B:2035:SER:OG   | 2.18                     | 0.59              |
| 4:F:2141:PRO:HB3  | 4:F:2228:ILE:HG21 | 1.83                     | 0.59              |
| 3:A:408:UNK:HB1   | 3:A:512:UNK:HA    | 1.84                     | 0.59              |
| 4:B:1752:LEU:HD21 | 4:B:1788:LYS:HG2  | 1.85                     | 0.59              |
| 4:F:2347:ASP:OD1  | 4:F:2350:SER:N    | 2.36                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1538:UNK:HG1  | 3:A:1563:UNK:HG1  | 1.84                     | 0.59              |
| 4:B:1673:LEU:HD22 | 4:B:1700:TYR:HB2  | 1.85                     | 0.59              |
| 6:D:8:VAL:HG11    | 6:D:36:ARG:HE     | 1.66                     | 0.59              |
| 4:F:2223:GLN:HE22 | 4:F:2352:LYS:HB2  | 1.68                     | 0.59              |
| 2:4:183:UNK:O     | 2:4:187:UNK:N     | 2.36                     | 0.59              |
| 2:2:183:UNK:O     | 2:2:187:UNK:N     | 2.36                     | 0.58              |
| 2:4:71:UNK:HA     | 2:4:74:UNK:HB2    | 1.85                     | 0.58              |
| 4:B:1901:GLN:HG3  | 4:B:2413:SER:HA   | 1.85                     | 0.58              |
| 4:B:2244:ASP:HB2  | 4:B:2249:LEU:HD11 | 1.85                     | 0.58              |
| 4:B:2256:LYS:HZ2  | 4:B:2257:LYS:HE3  | 1.66                     | 0.58              |
| 4:F:1490:TRP:CD1  | 4:F:1522:GLY:HA3  | 2.37                     | 0.58              |
| 6:H:8:VAL:HG11    | 6:H:36:ARG:HE     | 1.66                     | 0.58              |
| 2:2:71:UNK:HA     | 2:2:74:UNK:HB2    | 1.85                     | 0.58              |
| 1:3:440:UNK:HB2   | 1:3:444:UNK:N     | 2.18                     | 0.58              |
| 1:3:1509:UNK:HG3  | 1:3:1606:UNK:HG3  | 1.85                     | 0.58              |
| 4:B:1490:TRP:CD1  | 4:B:1522:GLY:HA3  | 2.38                     | 0.58              |
| 4:B:1430:ALA:O    | 4:B:1434:GLU:HG2  | 2.03                     | 0.58              |
| 6:D:138:PRO:HG2   | 6:D:182:ALA:HB2   | 1.83                     | 0.58              |
| 4:F:1430:ALA:O    | 4:F:1434:GLU:HG2  | 2.03                     | 0.58              |
| 4:F:1912:ASP:O    | 4:F:1950:ARG:NH1  | 2.37                     | 0.58              |
| 6:D:93:PHE:HE1    | 6:D:114:LEU:HD11  | 1.67                     | 0.58              |
| 4:F:2245:THR:HB   | 4:F:2342:SER:HA   | 1.85                     | 0.58              |
| 5:G:62:UNK:HG1    | 5:G:74:UNK:HB1    | 1.85                     | 0.58              |
| 3:E:1117:UNK:HB2  | 3:E:1410:UNK:HB2  | 1.86                     | 0.58              |
| 4:F:1901:GLN:HG3  | 4:F:2413:SER:HA   | 1.85                     | 0.58              |
| 1:1:2201:UNK:HG2  | 1:1:2202:UNK:HG3  | 1.84                     | 0.58              |
| 3:A:1117:UNK:HB2  | 3:A:1410:UNK:HB2  | 1.85                     | 0.58              |
| 3:E:408:UNK:HB1   | 3:E:512:UNK:HA    | 1.84                     | 0.58              |
| 6:H:184:TYR:OH    | 6:H:213:LYS:NZ    | 2.35                     | 0.58              |
| 1:1:1114:UNK:HB1  | 1:1:1315:UNK:HG1  | 1.84                     | 0.58              |
| 2:2:118:UNK:HG1   | 2:2:159:UNK:HG2   | 1.86                     | 0.58              |
| 4:B:1622:ARG:HB3  | 4:B:1622:ARG:CZ   | 2.33                     | 0.58              |
| 4:F:1673:LEU:HD22 | 4:F:1700:TYR:HB2  | 1.85                     | 0.58              |
| 4:F:1752:LEU:HD21 | 4:F:1788:LYS:HG2  | 1.85                     | 0.58              |
| 6:H:93:PHE:HE1    | 6:H:114:LEU:HD11  | 1.68                     | 0.58              |
| 1:1:1306:UNK:HG1  | 1:1:1508:UNK:HA   | 1.86                     | 0.58              |
| 5:C:54:UNK:HG3    | 7:C:999:RAP:H472  | 1.84                     | 0.58              |
| 6:D:181:ASP:OD2   | 6:D:232:SER:OG    | 2.18                     | 0.58              |
| 2:2:541:UNK:HG3   | 2:2:545:UNK:HB2   | 1.86                     | 0.58              |
| 1:3:21:UNK:O      | 1:3:25:UNK:HB2    | 2.04                     | 0.58              |
| 1:3:410:UNK:HA    | 1:3:413:UNK:HB2   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3:1306:UNK:HG1  | 1:3:1508:UNK:HA   | 1.86                     | 0.58              |
| 3:A:917:UNK:HG3   | 3:A:958:UNK:HG1   | 1.85                     | 0.58              |
| 4:F:1593:CYS:HA   | 4:F:1596:LEU:HD12 | 1.86                     | 0.58              |
| 1:1:80:UNK:HG3    | 1:1:82:UNK:HB1    | 1.85                     | 0.57              |
| 1:1:1509:UNK:HG3  | 1:1:1606:UNK:HG3  | 1.86                     | 0.57              |
| 4:B:2223:GLN:HE22 | 4:B:2352:LYS:HB2  | 1.67                     | 0.57              |
| 4:B:2245:THR:HB   | 4:B:2342:SER:HA   | 1.85                     | 0.57              |
| 6:H:76:ASN:HB3    | 6:H:77:PRO:HD2    | 1.86                     | 0.57              |
| 1:1:21:UNK:O      | 1:1:25:UNK:HB2    | 2.04                     | 0.57              |
| 4:B:1581:GLU:HB3  | 4:B:1585:ARG:HB2  | 1.86                     | 0.57              |
| 4:B:2264:GLU:HG3  | 4:B:2294:THR:HG21 | 1.86                     | 0.57              |
| 5:C:62:UNK:HG1    | 5:C:74:UNK:HB1    | 1.85                     | 0.57              |
| 5:G:54:UNK:HG3    | 7:G:999:RAP:H472  | 1.84                     | 0.57              |
| 1:3:7:UNK:O       | 1:3:11:UNK:N      | 2.38                     | 0.57              |
| 1:3:1114:UNK:HB1  | 1:3:1315:UNK:HG1  | 1.85                     | 0.57              |
| 3:A:407:UNK:HG2   | 3:A:410:UNK:HB2   | 1.87                     | 0.57              |
| 1:3:1809:UNK:HG1  | 1:3:2006:UNK:HG2  | 1.87                     | 0.57              |
| 1:1:1809:UNK:HG1  | 1:1:2006:UNK:HG2  | 1.86                     | 0.57              |
| 2:4:118:UNK:HG1   | 2:4:159:UNK:HG2   | 1.87                     | 0.57              |
| 2:4:541:UNK:HG3   | 2:4:545:UNK:HB2   | 1.86                     | 0.57              |
| 4:B:1644:VAL:HG13 | 4:B:1648:GLU:CD   | 2.30                     | 0.57              |
| 4:F:1581:GLU:HB3  | 4:F:1585:ARG:HB2  | 1.87                     | 0.57              |
| 3:A:1501:UNK:HG1  | 3:A:1544:UNK:HA   | 1.86                     | 0.57              |
| 4:F:1876:THR:HA   | 4:F:1879:MET:HE2  | 1.87                     | 0.57              |
| 1:1:114:UNK:O     | 1:1:117:UNK:HB2   | 2.05                     | 0.57              |
| 3:E:917:UNK:HG3   | 3:E:958:UNK:HG1   | 1.84                     | 0.57              |
| 3:E:1102:UNK:HA   | 3:E:1105:UNK:HB2  | 1.87                     | 0.57              |
| 3:E:1116:UNK:HG3  | 3:E:1392:UNK:HG3  | 1.87                     | 0.57              |
| 1:1:440:UNK:HB2   | 1:1:444:UNK:N     | 2.18                     | 0.57              |
| 2:2:513:UNK:HG1   | 2:2:550:UNK:HB1   | 1.86                     | 0.57              |
| 1:3:8:UNK:HG3     | 4:B:1568:ARG:HE   | 1.70                     | 0.57              |
| 1:3:94:UNK:O      | 1:3:96:UNK:N      | 2.38                     | 0.57              |
| 4:B:2101:TRP:HA   | 4:B:2104:TYR:HB2  | 1.87                     | 0.57              |
| 4:B:1912:ASP:O    | 4:B:1950:ARG:NH1  | 2.38                     | 0.57              |
| 4:B:1939:ILE:HA   | 4:B:1942:LEU:HD12 | 1.87                     | 0.57              |
| 6:D:76:ASN:HB3    | 6:D:77:PRO:HD2    | 1.87                     | 0.57              |
| 4:F:2244:ASP:HB2  | 4:F:2249:LEU:HD11 | 1.87                     | 0.57              |
| 1:3:2:UNK:H2      | 4:B:1622:ARG:NE   | 2.02                     | 0.56              |
| 1:3:80:UNK:HG3    | 1:3:82:UNK:HB1    | 1.86                     | 0.56              |
| 2:4:310:UNK:C     | 2:4:404:UNK:HB2   | 2.35                     | 0.56              |
| 4:B:1593:CYS:HA   | 4:B:1596:LEU:HD12 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:2264:GLU:HG3  | 4:F:2294:THR:HG21 | 1.86                     | 0.56              |
| 1:3:114:UNK:O     | 1:3:117:UNK:HB2   | 2.04                     | 0.56              |
| 3:E:407:UNK:HG2   | 3:E:410:UNK:HB2   | 1.87                     | 0.56              |
| 4:F:2321:THR:HG23 | 4:F:2387:MET:HG2  | 1.87                     | 0.56              |
| 4:F:2412:ASP:OD1  | 4:F:2412:ASP:N    | 2.36                     | 0.56              |
| 4:B:1899:ASN:ND2  | 4:B:1937:GLN:OE1  | 2.39                     | 0.56              |
| 4:B:2321:THR:HG23 | 4:B:2387:MET:HG2  | 1.87                     | 0.56              |
| 1:1:94:UNK:O      | 1:1:96:UNK:N      | 2.38                     | 0.56              |
| 1:3:1711:UNK:HG2  | 1:3:1911:UNK:HG1  | 1.87                     | 0.56              |
| 3:E:1501:UNK:HG1  | 3:E:1544:UNK:HA   | 1.86                     | 0.56              |
| 4:F:1939:ILE:HA   | 4:F:1942:LEU:HD12 | 1.87                     | 0.56              |
| 1:1:7:UNK:O       | 1:1:11:UNK:N      | 2.38                     | 0.56              |
| 1:1:8:UNK:HG3     | 4:F:1568:ARG:HE   | 1.69                     | 0.56              |
| 1:3:506:UNK:HA    | 1:3:509:UNK:HB2   | 1.88                     | 0.56              |
| 4:B:1513:ALA:HB1  | 4:B:1536:ILE:HG12 | 1.88                     | 0.56              |
| 3:E:1645:UNK:HG3  | 3:E:1655:UNK:HG2  | 1.88                     | 0.56              |
| 4:F:1591:VAL:O    | 4:F:1594:HIS:HB3  | 2.06                     | 0.56              |
| 4:F:2031:LEU:O    | 4:F:2035:SER:OG   | 2.18                     | 0.56              |
| 1:1:1711:UNK:HG2  | 1:1:1911:UNK:HG1  | 1.88                     | 0.56              |
| 2:4:307:UNK:HG2   | 2:4:407:UNK:HG1   | 1.87                     | 0.56              |
| 4:B:1600:GLU:O    | 4:B:1603:ILE:HG22 | 2.05                     | 0.56              |
| 3:E:549:UNK:HB1   | 3:E:554:UNK:HG2   | 1.88                     | 0.56              |
| 4:F:2101:TRP:HA   | 4:F:2104:TYR:HB2  | 1.87                     | 0.56              |
| 2:4:209:UNK:HB2   | 2:4:246:UNK:HB2   | 1.87                     | 0.56              |
| 3:A:949:UNK:HA    | 3:A:952:UNK:HB2   | 1.87                     | 0.56              |
| 3:A:1102:UNK:HA   | 3:A:1105:UNK:HB2  | 1.87                     | 0.56              |
| 3:A:1116:UNK:HG3  | 3:A:1392:UNK:HG3  | 1.88                     | 0.56              |
| 4:B:2310:SER:O    | 4:B:2313:TRP:HB3  | 2.06                     | 0.56              |
| 6:D:243:THR:HG21  | 6:D:245:LYS:HE3   | 1.88                     | 0.56              |
| 2:2:93:UNK:HG2    | 2:2:135:UNK:HB1   | 1.88                     | 0.56              |
| 3:A:575:UNK:O     | 3:A:578:UNK:HB2   | 2.06                     | 0.56              |
| 3:A:1645:UNK:HG3  | 3:A:1655:UNK:HG2  | 1.88                     | 0.56              |
| 4:F:1600:GLU:O    | 4:F:1603:ILE:HG22 | 2.05                     | 0.56              |
| 1:3:88:UNK:HG1    | 1:3:106:UNK:HA    | 1.87                     | 0.56              |
| 3:A:549:UNK:HB1   | 3:A:554:UNK:HG2   | 1.88                     | 0.56              |
| 4:B:1876:THR:HA   | 4:B:1879:MET:HE2  | 1.87                     | 0.56              |
| 2:2:310:UNK:C     | 2:2:404:UNK:HB2   | 2.35                     | 0.55              |
| 4:F:2534:SER:OG   | 4:F:2537:ASN:ND2  | 2.39                     | 0.55              |
| 1:1:88:UNK:HG1    | 1:1:106:UNK:HA    | 1.87                     | 0.55              |
| 4:B:2534:SER:OG   | 4:B:2537:ASN:ND2  | 2.39                     | 0.55              |
| 6:D:184:TYR:OH    | 6:D:213:LYS:NZ    | 2.35                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:1410:PRO:HA   | 4:F:1413:LEU:HD12 | 1.87                     | 0.55              |
| 4:F:1899:ASN:ND2  | 4:F:1937:GLN:OE1  | 2.38                     | 0.55              |
| 4:F:2419:GLU:OE2  | 4:F:2505:ARG:NH1  | 2.38                     | 0.55              |
| 1:1:506:UNK:HA    | 1:1:509:UNK:HB2   | 1.88                     | 0.55              |
| 3:E:949:UNK:HA    | 3:E:952:UNK:HB2   | 1.87                     | 0.55              |
| 4:F:1513:ALA:HB1  | 4:F:1536:ILE:HG12 | 1.89                     | 0.55              |
| 4:F:1619:TRP:CH2  | 4:F:1640:ARG:HB3  | 2.42                     | 0.55              |
| 4:F:1644:VAL:HG13 | 4:F:1648:GLU:CD   | 2.30                     | 0.55              |
| 1:1:2:UNK:H2      | 4:F:1622:ARG:NE   | 2.03                     | 0.55              |
| 1:1:410:UNK:HA    | 1:1:413:UNK:HB2   | 1.88                     | 0.55              |
| 4:B:1943:ILE:HA   | 4:B:1946:ILE:HG13 | 1.87                     | 0.55              |
| 4:B:2419:GLU:OE2  | 4:B:2505:ARG:NH1  | 2.39                     | 0.55              |
| 4:F:1943:ILE:HA   | 4:F:1946:ILE:HG13 | 1.87                     | 0.55              |
| 4:F:2156:ILE:HG12 | 4:F:2174:LEU:HD22 | 1.89                     | 0.55              |
| 4:B:1410:PRO:HA   | 4:B:1413:LEU:HD12 | 1.88                     | 0.55              |
| 4:B:1591:VAL:O    | 4:B:1594:HIS:HB3  | 2.06                     | 0.55              |
| 2:4:544:UNK:O     | 2:4:548:UNK:HG2   | 2.06                     | 0.55              |
| 3:A:617:UNK:HG1   | 3:A:633:UNK:HB2   | 1.88                     | 0.55              |
| 4:F:1474:PRO:HA   | 4:F:1477:MET:HE2  | 1.89                     | 0.55              |
| 1:3:120:UNK:HB1   | 1:3:123:UNK:HB2   | 1.89                     | 0.55              |
| 3:E:1395:UNK:O    | 3:E:1408:UNK:N    | 2.40                     | 0.55              |
| 1:1:44:UNK:HA     | 1:1:47:UNK:CB     | 2.38                     | 0.54              |
| 5:C:27:UNK:HG2    | 5:C:100:UNK:HB2   | 1.89                     | 0.54              |
| 2:2:544:UNK:O     | 2:2:548:UNK:HG2   | 2.06                     | 0.54              |
| 1:3:416:UNK:O     | 1:3:418:UNK:N     | 2.26                     | 0.54              |
| 4:B:2156:ILE:HG12 | 4:B:2174:LEU:HD22 | 1.89                     | 0.54              |
| 3:E:575:UNK:O     | 3:E:578:UNK:HB2   | 2.06                     | 0.54              |
| 6:H:159:THR:OG1   | 6:H:206:GLU:OE1   | 2.25                     | 0.54              |
| 1:1:88:UNK:HA     | 1:1:91:UNK:HB2    | 1.89                     | 0.54              |
| 2:2:307:UNK:HG2   | 2:2:407:UNK:HG1   | 1.87                     | 0.54              |
| 1:3:49:UNK:O      | 1:3:52:UNK:HG3    | 2.08                     | 0.54              |
| 2:4:192:UNK:HA    | 2:4:195:UNK:HB2   | 1.89                     | 0.54              |
| 4:B:1619:TRP:CH2  | 4:B:1640:ARG:HB3  | 2.42                     | 0.54              |
| 4:B:2184:PHE:HB3  | 4:B:2236:LEU:HD22 | 1.88                     | 0.54              |
| 6:D:288:ALA:HB1   | 6:D:315:VAL:HG12  | 1.89                     | 0.54              |
| 3:E:617:UNK:HG1   | 3:E:633:UNK:HB2   | 1.89                     | 0.54              |
| 3:E:985:UNK:HB1   | 3:E:988:UNK:HB2   | 1.89                     | 0.54              |
| 2:4:93:UNK:HG2    | 2:4:135:UNK:HB1   | 1.89                     | 0.54              |
| 4:F:2327:MET:HE2  | 4:F:2355:HIS:HB2  | 1.90                     | 0.54              |
| 5:G:27:UNK:HG2    | 5:G:100:UNK:HB2   | 1.89                     | 0.54              |
| 1:1:49:UNK:O      | 1:1:52:UNK:HG3    | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:239:UNK:O     | 2:2:243:UNK:HB2   | 2.07                     | 0.54              |
| 3:A:1395:UNK:O    | 3:A:1408:UNK:N    | 2.41                     | 0.54              |
| 4:B:1653:TRP:HB2  | 4:B:1676:LEU:HD11 | 1.90                     | 0.54              |
| 4:F:1445:ILE:HG13 | 4:F:1449:TRP:CZ3  | 2.43                     | 0.54              |
| 6:H:243:THR:HG21  | 6:H:245:LYS:HE3   | 1.88                     | 0.54              |
| 2:2:82:UNK:HA     | 2:2:85:UNK:HB2    | 1.88                     | 0.54              |
| 4:B:1938:VAL:HG13 | 4:B:1942:LEU:HG   | 1.89                     | 0.54              |
| 4:F:2265:HIS:HA   | 4:F:2268:MET:SD   | 2.48                     | 0.54              |
| 1:1:1:UNK:O       | 1:1:5:UNK:N       | 2.41                     | 0.54              |
| 1:1:31:UNK:O      | 1:1:36:UNK:HB2    | 2.08                     | 0.54              |
| 1:1:416:UNK:C     | 1:1:418:UNK:H     | 2.16                     | 0.54              |
| 2:2:192:UNK:HA    | 2:2:195:UNK:HB2   | 1.89                     | 0.54              |
| 2:4:239:UNK:O     | 2:4:243:UNK:HB2   | 2.07                     | 0.54              |
| 4:F:1622:ARG:HB3  | 4:F:1622:ARG:CZ   | 2.34                     | 0.54              |
| 1:3:31:UNK:O      | 1:3:36:UNK:HB2    | 2.08                     | 0.54              |
| 3:A:985:UNK:HB1   | 3:A:988:UNK:HB2   | 1.89                     | 0.54              |
| 3:A:1628:UNK:HB1  | 3:A:1648:UNK:HG1  | 1.90                     | 0.54              |
| 4:B:2327:MET:HE2  | 4:B:2355:HIS:HB2  | 1.89                     | 0.54              |
| 4:B:2393:ASP:OD1  | 4:B:2397:ARG:NH1  | 2.41                     | 0.54              |
| 4:F:2304:TRP:HA   | 4:F:2313:TRP:CD1  | 2.43                     | 0.54              |
| 6:H:98:ARG:HG3    | 6:H:115:ARG:HD2   | 1.90                     | 0.54              |
| 4:B:2324:LEU:O    | 4:B:2328:SER:OG   | 2.17                     | 0.53              |
| 6:D:159:THR:OG1   | 6:D:206:GLU:OE1   | 2.25                     | 0.53              |
| 3:E:1311:UNK:HB2  | 3:E:1664:UNK:HB2  | 1.89                     | 0.53              |
| 4:F:2038:TYR:HE1  | 4:F:2044:VAL:HG22 | 1.73                     | 0.53              |
| 1:1:44:UNK:HA     | 1:1:47:UNK:HB2    | 1.90                     | 0.53              |
| 2:4:117:UNK:O     | 2:4:119:UNK:N     | 2.42                     | 0.53              |
| 3:A:1311:UNK:HB2  | 3:A:1664:UNK:HB2  | 1.89                     | 0.53              |
| 4:B:2038:TYR:HE1  | 4:B:2044:VAL:HG22 | 1.73                     | 0.53              |
| 4:F:2184:PHE:HB3  | 4:F:2236:LEU:HD22 | 1.89                     | 0.53              |
| 4:F:2310:SER:O    | 4:F:2313:TRP:HB3  | 2.07                     | 0.53              |
| 6:H:40:HIS:HE1    | 6:H:43:SER:HB3    | 1.74                     | 0.53              |
| 4:B:1474:PRO:HA   | 4:B:1477:MET:HE2  | 1.89                     | 0.53              |
| 4:B:2304:TRP:HA   | 4:B:2313:TRP:CD1  | 2.43                     | 0.53              |
| 6:D:14:ILE:HD13   | 6:D:70:LEU:HD13   | 1.91                     | 0.53              |
| 1:1:334:UNK:HB2   | 1:1:402:UNK:HB2   | 1.90                     | 0.53              |
| 1:3:88:UNK:HA     | 1:3:91:UNK:HB2    | 1.91                     | 0.53              |
| 4:B:1598:GLU:OE2  | 4:B:1619:TRP:NE1  | 2.42                     | 0.53              |
| 6:D:32:GLY:HA2    | 6:D:308:TYR:CD2   | 2.42                     | 0.53              |
| 3:E:517:UNK:O     | 3:E:519:UNK:N     | 2.42                     | 0.53              |
| 4:F:1598:GLU:OE2  | 4:F:1619:TRP:NE1  | 2.41                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:F:1621:GLU:O   | 4:F:1625:GLY:N    | 2.42                     | 0.53              |
| 2:2:197:UNK:O    | 2:2:201:UNK:N     | 2.42                     | 0.53              |
| 1:3:334:UNK:HB2  | 1:3:402:UNK:HB2   | 1.89                     | 0.53              |
| 4:B:2411:LYS:HB2 | 4:B:2508:LEU:HD13 | 1.90                     | 0.53              |
| 4:F:1581:GLU:HB3 | 4:F:1585:ARG:H    | 1.74                     | 0.53              |
| 4:F:1653:TRP:HB2 | 4:F:1676:LEU:HD11 | 1.89                     | 0.53              |
| 1:1:42:UNK:O     | 1:1:45:UNK:HB2    | 2.09                     | 0.53              |
| 1:3:44:UNK:HA    | 1:3:47:UNK:HB2    | 1.90                     | 0.53              |
| 1:3:48:UNK:HA    | 1:3:51:UNK:HG3    | 1.91                     | 0.53              |
| 4:B:1514:ARG:HA  | 4:B:1536:ILE:HD13 | 1.91                     | 0.53              |
| 6:D:98:ARG:HG3   | 6:D:115:ARG:HD2   | 1.90                     | 0.53              |
| 4:F:1947:ASP:HB3 | 4:F:1987:ARG:HG2  | 1.91                     | 0.53              |
| 3:E:1628:UNK:HB1 | 3:E:1648:UNK:HG1  | 1.90                     | 0.53              |
| 6:H:288:ALA:HB1  | 6:H:315:VAL:HG12  | 1.89                     | 0.53              |
| 1:3:44:UNK:HA    | 1:3:47:UNK:CB     | 2.38                     | 0.53              |
| 4:B:1590:MET:HA  | 4:B:1593:CYS:SG   | 2.48                     | 0.53              |
| 4:B:1704:MET:HE3 | 4:B:1713:ALA:HA   | 1.91                     | 0.53              |
| 6:D:40:HIS:HE1   | 6:D:43:SER:HB3    | 1.74                     | 0.53              |
| 6:H:14:ILE:HD13  | 6:H:70:LEU:HD13   | 1.91                     | 0.53              |
| 1:1:61:UNK:O     | 1:1:64:UNK:HB2    | 2.09                     | 0.52              |
| 1:1:120:UNK:HB1  | 1:1:123:UNK:HB2   | 1.90                     | 0.52              |
| 1:3:1:UNK:O      | 1:3:5:UNK:N       | 2.41                     | 0.52              |
| 1:3:42:UNK:O     | 1:3:45:UNK:HB2    | 2.09                     | 0.52              |
| 1:3:61:UNK:O     | 1:3:64:UNK:HB2    | 2.09                     | 0.52              |
| 2:4:259:UNK:HA   | 2:4:262:UNK:HG3   | 1.92                     | 0.52              |
| 4:B:2265:HIS:HA  | 4:B:2268:MET:SD   | 2.48                     | 0.52              |
| 3:E:1347:UNK:HG3 | 3:E:1359:UNK:HG2  | 1.91                     | 0.52              |
| 4:F:2411:LYS:HB2 | 4:F:2508:LEU:HD13 | 1.90                     | 0.52              |
| 3:A:517:UNK:O    | 3:A:519:UNK:N     | 2.42                     | 0.52              |
| 7:C:999:RAP:H432 | 7:C:999:RAP:O4    | 2.09                     | 0.52              |
| 4:F:1590:MET:HA  | 4:F:1593:CYS:SG   | 2.48                     | 0.52              |
| 1:1:304:UNK:CB   | 2:2:71:UNK:HB1    | 2.39                     | 0.52              |
| 1:3:1510:UNK:HG2 | 1:3:1712:UNK:HG1  | 1.90                     | 0.52              |
| 2:4:197:UNK:O    | 2:4:201:UNK:N     | 2.41                     | 0.52              |
| 3:A:1347:UNK:HG3 | 3:A:1359:UNK:HG2  | 1.92                     | 0.52              |
| 4:B:2251:ARG:HA  | 4:B:2261:LEU:HD13 | 1.91                     | 0.52              |
| 4:B:2268:MET:HE1 | 4:B:2543:ILE:HD11 | 1.92                     | 0.52              |
| 3:E:320:UNK:HA   | 3:E:331:UNK:HA    | 1.92                     | 0.52              |
| 3:E:967:UNK:HB2  | 3:E:969:UNK:HG2   | 1.91                     | 0.52              |
| 4:F:2298:ASP:HB2 | 4:F:2382:MET:SD   | 2.49                     | 0.52              |
| 4:F:2393:ASP:OD1 | 4:F:2397:ARG:NH1  | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1510:UNK:HG2  | 1:1:1712:UNK:HG1  | 1.90                     | 0.52              |
| 4:F:1446:GLN:O    | 4:F:1449:TRP:HB2  | 2.09                     | 0.52              |
| 4:F:1938:VAL:HG13 | 4:F:1942:LEU:HG   | 1.90                     | 0.52              |
| 4:F:1977:THR:O    | 4:F:1980:SER:OG   | 2.27                     | 0.52              |
| 3:A:727:UNK:HG2   | 3:A:766:UNK:HG1   | 1.92                     | 0.52              |
| 4:B:1417:ILE:HG23 | 4:B:1432:VAL:HB   | 1.92                     | 0.52              |
| 4:F:2506:ASP:O    | 4:F:2511:ARG:N    | 2.37                     | 0.52              |
| 1:1:446:UNK:HA    | 1:1:449:UNK:HB2   | 1.92                     | 0.52              |
| 2:2:269:UNK:HG3   | 2:2:400:UNK:HA    | 1.91                     | 0.52              |
| 4:B:1621:GLU:O    | 4:B:1625:GLY:N    | 2.42                     | 0.52              |
| 4:B:2298:ASP:HB2  | 4:B:2382:MET:SD   | 2.49                     | 0.52              |
| 6:D:16:ALA:HB3    | 6:D:319:ALA:HB3   | 1.92                     | 0.52              |
| 4:F:1514:ARG:HA   | 4:F:1536:ILE:HD13 | 1.91                     | 0.52              |
| 4:F:2036:ARG:HA   | 7:G:999:RAP:H521  | 1.92                     | 0.52              |
| 4:F:2290:ALA:O    | 4:F:2294:THR:OG1  | 2.19                     | 0.52              |
| 1:1:1700:UNK:HB1  | 1:1:1900:UNK:HB2  | 1.91                     | 0.52              |
| 1:3:446:UNK:HA    | 1:3:449:UNK:HB2   | 1.91                     | 0.52              |
| 3:A:1383:UNK:HG3  | 3:A:1397:UNK:HA   | 1.92                     | 0.52              |
| 4:B:1484:LEU:HA   | 4:B:1487:LEU:HB2  | 1.92                     | 0.52              |
| 1:3:422:UNK:C     | 1:3:424:UNK:H     | 2.22                     | 0.52              |
| 2:4:82:UNK:HA     | 2:4:85:UNK:HB2    | 1.91                     | 0.52              |
| 2:4:269:UNK:HG3   | 2:4:400:UNK:HA    | 1.92                     | 0.52              |
| 4:B:1413:LEU:HD22 | 4:B:1436:ALA:HB2  | 1.92                     | 0.52              |
| 4:B:1947:ASP:HB3  | 4:B:1987:ARG:HG2  | 1.91                     | 0.52              |
| 4:B:2346:LEU:HD23 | 4:B:2353:ILE:HG13 | 1.92                     | 0.52              |
| 6:D:132:ASN:HD21  | 6:D:148:GLN:HG2   | 1.74                     | 0.52              |
| 3:E:247:UNK:HA    | 3:E:250:UNK:HB1   | 1.92                     | 0.52              |
| 4:F:2268:MET:HE1  | 4:F:2543:ILE:HD11 | 1.92                     | 0.52              |
| 1:1:159:UNK:HB1   | 1:1:200:UNK:HB1   | 1.92                     | 0.52              |
| 4:B:2045:LYS:NZ   | 4:B:2049:GLU:OE2  | 2.43                     | 0.52              |
| 4:F:1413:LEU:HD22 | 4:F:1436:ALA:HB2  | 1.92                     | 0.52              |
| 4:F:1632:ASP:O    | 4:F:1636:ILE:HD13 | 2.10                     | 0.52              |
| 6:H:19:GLY:HA3    | 6:H:314:ALA:O     | 2.10                     | 0.52              |
| 2:2:71:UNK:O      | 2:2:75:UNK:N      | 2.43                     | 0.52              |
| 1:3:809:UNK:HG3   | 1:3:903:UNK:HG3   | 1.92                     | 0.52              |
| 3:A:967:UNK:HB2   | 3:A:969:UNK:HG2   | 1.92                     | 0.52              |
| 3:A:1592:UNK:HB1  | 3:A:1604:UNK:HA   | 1.92                     | 0.52              |
| 4:B:1446:GLN:O    | 4:B:1449:TRP:HB2  | 2.10                     | 0.52              |
| 4:B:1632:ASP:O    | 4:B:1636:ILE:HD13 | 2.10                     | 0.52              |
| 4:B:1918:ASP:OD1  | 4:B:1918:ASP:N    | 2.42                     | 0.52              |
| 4:F:1417:ILE:HG23 | 4:F:1432:VAL:HB   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:422:UNK:C     | 1:1:424:UNK:H     | 2.22                     | 0.51              |
| 4:B:2024:HIS:CD2  | 4:B:2025:GLU:HG3  | 2.46                     | 0.51              |
| 4:B:2282:GLN:HG3  | 6:D:274:TRP:CH2   | 2.45                     | 0.51              |
| 4:B:2515:HIS:ND1  | 4:B:2516:ASP:OD1  | 2.43                     | 0.51              |
| 4:F:1484:LEU:HA   | 4:F:1487:LEU:HB2  | 1.92                     | 0.51              |
| 4:F:2264:GLU:O    | 4:F:2268:MET:HG3  | 2.10                     | 0.51              |
| 1:1:48:UNK:HA     | 1:1:51:UNK:HG3    | 1.90                     | 0.51              |
| 4:B:2412:ASP:OD1  | 4:B:2412:ASP:N    | 2.36                     | 0.51              |
| 6:D:40:HIS:CD2    | 6:D:66:ARG:HD2    | 2.45                     | 0.51              |
| 3:E:1383:UNK:HG3  | 3:E:1397:UNK:HA   | 1.92                     | 0.51              |
| 4:F:1918:ASP:OD1  | 4:F:1918:ASP:N    | 2.43                     | 0.51              |
| 7:G:999:RAP:O4    | 7:G:999:RAP:H432  | 2.09                     | 0.51              |
| 6:H:195:TYR:CZ    | 6:H:215:LYS:HG3   | 2.45                     | 0.51              |
| 2:2:187:UNK:O     | 2:2:191:UNK:HG2   | 2.10                     | 0.51              |
| 2:2:259:UNK:HA    | 2:2:262:UNK:HG3   | 1.92                     | 0.51              |
| 2:2:617:UNK:HA    | 4:B:1393:TYR:CE1  | 2.46                     | 0.51              |
| 1:3:1103:UNK:O    | 1:3:1107:UNK:HB2  | 2.10                     | 0.51              |
| 1:3:1700:UNK:HB1  | 1:3:1900:UNK:HB2  | 1.91                     | 0.51              |
| 2:4:71:UNK:O      | 2:4:75:UNK:N      | 2.43                     | 0.51              |
| 3:A:1731:UNK:O    | 3:A:1732:UNK:HB2  | 2.11                     | 0.51              |
| 4:B:1749:ARG:HG2  | 4:B:1786:TRP:HH2  | 1.74                     | 0.51              |
| 4:F:1704:MET:HE3  | 4:F:1713:ALA:HA   | 1.91                     | 0.51              |
| 4:F:1749:ARG:HG2  | 4:F:1786:TRP:HH2  | 1.74                     | 0.51              |
| 4:F:2251:ARG:HA   | 4:F:2261:LEU:HD13 | 1.92                     | 0.51              |
| 4:F:2267:ILE:HA   | 4:F:2270:ARG:HB3  | 1.92                     | 0.51              |
| 4:F:2346:LEU:HD23 | 4:F:2353:ILE:HG13 | 1.92                     | 0.51              |
| 1:1:1004:UNK:HG1  | 1:1:1104:UNK:HA   | 1.93                     | 0.51              |
| 2:4:617:UNK:HA    | 4:F:1393:TYR:CE1  | 2.45                     | 0.51              |
| 3:A:210:UNK:O     | 3:A:212:UNK:N     | 2.44                     | 0.51              |
| 3:A:217:UNK:O     | 3:A:221:UNK:HG2   | 2.10                     | 0.51              |
| 4:B:1568:ARG:HG2  | 4:B:1596:LEU:HD13 | 1.91                     | 0.51              |
| 3:E:211:UNK:HB1   | 4:F:2118:LEU:HA   | 1.93                     | 0.51              |
| 3:E:217:UNK:O     | 3:E:221:UNK:HG2   | 2.10                     | 0.51              |
| 3:E:405:UNK:HG1   | 3:E:413:UNK:HG1   | 1.92                     | 0.51              |
| 3:E:1592:UNK:HB1  | 3:E:1604:UNK:HA   | 1.92                     | 0.51              |
| 4:B:1581:GLU:HB3  | 4:B:1585:ARG:H    | 1.76                     | 0.51              |
| 4:B:2267:ILE:HA   | 4:B:2270:ARG:HB3  | 1.92                     | 0.51              |
| 4:F:2023:TRP:HE1  | 4:F:2057:MET:HE3  | 1.74                     | 0.51              |
| 4:F:2401:HIS:HA   | 4:F:2521:VAL:CG1  | 2.41                     | 0.51              |
| 1:1:809:UNK:HG3   | 1:1:903:UNK:HG3   | 1.91                     | 0.51              |
| 2:2:117:UNK:O     | 2:2:119:UNK:N     | 2.43                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:4:187:UNK:O    | 2:4:191:UNK:HG2   | 2.10                     | 0.51              |
| 4:B:2506:ASP:O   | 4:B:2511:ARG:N    | 2.37                     | 0.51              |
| 6:D:111:ILE:HD12 | 6:D:123:ARG:HD3   | 1.92                     | 0.51              |
| 4:F:2336:LEU:HG  | 4:F:2339:ARG:HD2  | 1.93                     | 0.51              |
| 6:H:32:GLY:HA2   | 6:H:308:TYR:CD2   | 2.43                     | 0.51              |
| 6:H:40:HIS:CD2   | 6:H:66:ARG:HD2    | 2.45                     | 0.51              |
| 1:3:304:UNK:CB   | 2:4:71:UNK:HB1    | 2.40                     | 0.51              |
| 3:A:247:UNK:HA   | 3:A:250:UNK:HB1   | 1.92                     | 0.51              |
| 3:E:1609:UNK:HG2 | 3:E:1632:UNK:HB1  | 1.92                     | 0.51              |
| 3:E:1731:UNK:O   | 3:E:1732:UNK:HB2  | 2.11                     | 0.51              |
| 1:1:92:UNK:HA    | 1:1:94:UNK:HG2    | 1.93                     | 0.51              |
| 1:3:92:UNK:HA    | 1:3:94:UNK:HG2    | 1.93                     | 0.51              |
| 1:3:416:UNK:C    | 1:3:418:UNK:H     | 2.17                     | 0.51              |
| 4:B:2401:HIS:HA  | 4:B:2521:VAL:CG1  | 2.40                     | 0.51              |
| 6:H:16:ALA:HB3   | 6:H:319:ALA:HB3   | 1.91                     | 0.51              |
| 1:1:435:UNK:HG1  | 1:1:447:UNK:HG1   | 1.93                     | 0.51              |
| 2:2:126:UNK:HB1  | 2:2:169:UNK:HB2   | 1.93                     | 0.51              |
| 4:F:2038:TYR:CE1 | 4:F:2044:VAL:HG22 | 2.46                     | 0.51              |
| 1:1:327:UNK:O    | 1:1:330:UNK:HG2   | 2.11                     | 0.50              |
| 1:1:1103:UNK:O   | 1:1:1107:UNK:HB2  | 2.11                     | 0.50              |
| 2:2:141:UNK:HG3  | 2:2:179:UNK:HG1   | 1.93                     | 0.50              |
| 2:4:141:UNK:HG3  | 2:4:179:UNK:HG1   | 1.93                     | 0.50              |
| 4:B:2036:ARG:HA  | 7:C:999:RAP:H521  | 1.92                     | 0.50              |
| 4:B:2336:LEU:HG  | 4:B:2339:ARG:HD2  | 1.93                     | 0.50              |
| 6:D:167:PRO:HG3  | 6:D:197:TRP:CZ2   | 2.46                     | 0.50              |
| 6:D:195:TYR:CZ   | 6:D:215:LYS:HG3   | 2.46                     | 0.50              |
| 4:F:2012:VAL:O   | 4:F:2016:LEU:HG   | 2.12                     | 0.50              |
| 4:F:2282:GLN:HG3 | 6:H:274:TRP:CH2   | 2.46                     | 0.50              |
| 1:3:1004:UNK:HG1 | 1:3:1104:UNK:HA   | 1.93                     | 0.50              |
| 2:4:181:UNK:HA   | 2:4:184:UNK:HG2   | 1.93                     | 0.50              |
| 3:A:320:UNK:HA   | 3:A:331:UNK:HA    | 1.92                     | 0.50              |
| 3:A:1609:UNK:HG2 | 3:A:1632:UNK:HB1  | 1.92                     | 0.50              |
| 6:D:17:THR:HB    | 6:D:27:TRP:HE1    | 1.77                     | 0.50              |
| 6:D:19:GLY:HA3   | 6:D:314:ALA:O     | 2.10                     | 0.50              |
| 3:E:210:UNK:O    | 3:E:212:UNK:N     | 2.44                     | 0.50              |
| 3:E:894:UNK:HA   | 3:E:937:UNK:HG1   | 1.93                     | 0.50              |
| 1:3:327:UNK:O    | 1:3:330:UNK:HG2   | 2.11                     | 0.50              |
| 4:B:1688:PRO:HA  | 4:B:1716:HIS:CE1  | 2.47                     | 0.50              |
| 4:B:2023:TRP:HE1 | 4:B:2057:MET:HE3  | 1.76                     | 0.50              |
| 4:B:2415:MET:HE1 | 4:B:2501:ILE:HG23 | 1.94                     | 0.50              |
| 2:4:180:UNK:O    | 2:4:183:UNK:N     | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:2270:ARG:O    | 6:D:313:LYS:NZ    | 2.27                     | 0.50              |
| 4:F:1907:LEU:HD13 | 4:F:1911:PHE:CZ   | 2.46                     | 0.50              |
| 4:F:2024:HIS:CD2  | 4:F:2025:GLU:HG3  | 2.46                     | 0.50              |
| 1:1:416:UNK:O     | 1:1:418:UNK:N     | 2.27                     | 0.50              |
| 1:3:210:UNK:O     | 1:3:212:UNK:N     | 2.45                     | 0.50              |
| 1:3:1805:UNK:HG1  | 1:3:2003:UNK:HG1  | 1.93                     | 0.50              |
| 2:4:104:UNK:O     | 2:4:108:UNK:HB2   | 2.12                     | 0.50              |
| 4:B:1557:PHE:HD1  | 4:B:1603:ILE:HG13 | 1.77                     | 0.50              |
| 4:B:1907:LEU:HD13 | 4:B:1911:PHE:CZ   | 2.46                     | 0.50              |
| 4:B:1973:ILE:HG21 | 4:B:2005:LEU:HD13 | 1.93                     | 0.50              |
| 4:B:2139:ALA:HA   | 4:B:2152:ARG:HA   | 1.94                     | 0.50              |
| 3:E:1509:UNK:O    | 3:E:1525:UNK:N    | 2.45                     | 0.50              |
| 4:F:1529:MET:O    | 4:F:1533:THR:OG1  | 2.16                     | 0.50              |
| 4:F:1631:GLU:OE2  | 4:F:1665:ARG:NH2  | 2.45                     | 0.50              |
| 6:H:132:ASN:HD21  | 6:H:148:GLN:HG2   | 1.74                     | 0.50              |
| 4:B:1571:LEU:HD21 | 4:B:1589:ALA:HB1  | 1.94                     | 0.50              |
| 4:B:2038:TYR:CE1  | 4:B:2044:VAL:HG22 | 2.46                     | 0.50              |
| 4:F:1688:PRO:HA   | 4:F:1716:HIS:CE1  | 2.47                     | 0.50              |
| 2:2:180:UNK:O     | 2:2:183:UNK:N     | 2.44                     | 0.50              |
| 4:F:1568:ARG:HG2  | 4:F:1596:LEU:HD13 | 1.92                     | 0.50              |
| 4:F:1571:LEU:HD21 | 4:F:1589:ALA:HB1  | 1.94                     | 0.50              |
| 4:F:1581:GLU:HB2  | 4:F:1585:ARG:HB2  | 1.94                     | 0.50              |
| 2:2:549:UNK:O     | 2:2:552:UNK:HG3   | 2.12                     | 0.50              |
| 1:3:159:UNK:HB1   | 1:3:200:UNK:HB1   | 1.93                     | 0.50              |
| 4:B:1910:TRP:HZ2  | 4:B:1956:LEU:HB3  | 1.77                     | 0.50              |
| 5:C:25:UNK:HA     | 5:C:39:UNK:HG1    | 1.93                     | 0.50              |
| 4:F:1591:VAL:HG13 | 4:F:1636:ILE:HD11 | 1.93                     | 0.50              |
| 4:F:1973:ILE:HG21 | 4:F:2005:LEU:HD13 | 1.93                     | 0.50              |
| 4:F:2415:MET:HE1  | 4:F:2501:ILE:HG23 | 1.93                     | 0.50              |
| 6:H:111:ILE:HD12  | 6:H:123:ARG:HD3   | 1.92                     | 0.50              |
| 6:H:242:GLN:OE1   | 6:H:270:ARG:N     | 2.45                     | 0.50              |
| 2:2:183:UNK:HA    | 2:2:186:UNK:HB1   | 1.93                     | 0.49              |
| 3:A:211:UNK:HB1   | 4:B:2118:LEU:HA   | 1.94                     | 0.49              |
| 3:A:405:UNK:HG1   | 3:A:413:UNK:HG1   | 1.92                     | 0.49              |
| 4:B:2012:VAL:O    | 4:B:2016:LEU:HG   | 2.12                     | 0.49              |
| 3:E:1509:UNK:HB1  | 3:E:1525:UNK:HB2  | 1.93                     | 0.49              |
| 1:3:304:UNK:HB2   | 2:4:71:UNK:HB1    | 1.95                     | 0.49              |
| 4:B:1417:ILE:HG22 | 4:B:1429:ALA:HB1  | 1.94                     | 0.49              |
| 4:B:2264:GLU:O    | 4:B:2268:MET:HG3  | 2.11                     | 0.49              |
| 3:E:1512:UNK:HG1  | 3:E:1555:UNK:HG1  | 1.95                     | 0.49              |
| 4:F:1557:PHE:HD1  | 4:F:1603:ILE:HG13 | 1.77                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:G:25:UNK:HA     | 5:G:39:UNK:HG1   | 1.93                     | 0.49              |
| 5:G:77:UNK:HA     | 5:G:96:UNK:HG3   | 1.93                     | 0.49              |
| 2:4:160:UNK:HG1   | 2:4:197:UNK:HB2  | 1.93                     | 0.49              |
| 3:A:559:UNK:HB2   | 3:A:566:UNK:HB2  | 1.93                     | 0.49              |
| 3:A:1512:UNK:HG1  | 3:A:1555:UNK:HG1 | 1.94                     | 0.49              |
| 6:D:293:LEU:HD12  | 6:D:295:ARG:NH2  | 2.27                     | 0.49              |
| 4:F:2408:ARG:O    | 4:F:2411:LYS:HG2 | 2.13                     | 0.49              |
| 6:H:293:LEU:HD12  | 6:H:295:ARG:NH2  | 2.27                     | 0.49              |
| 1:1:210:UNK:O     | 1:1:212:UNK:N    | 2.45                     | 0.49              |
| 2:2:104:UNK:O     | 2:2:108:UNK:HB2  | 2.12                     | 0.49              |
| 1:3:120:UNK:O     | 1:3:124:UNK:N    | 2.46                     | 0.49              |
| 3:A:827:UNK:HG1   | 3:A:875:UNK:HG1  | 1.95                     | 0.49              |
| 4:B:1702:LYS:HG3  | 4:B:1706:LYS:HE3 | 1.95                     | 0.49              |
| 4:B:2279:THR:N    | 4:B:2282:GLN:OE1 | 2.40                     | 0.49              |
| 3:E:559:UNK:HB2   | 3:E:566:UNK:HB2  | 1.93                     | 0.49              |
| 4:F:1605:TYR:O    | 4:F:1612:ARG:NH1 | 2.46                     | 0.49              |
| 4:F:2515:HIS:ND1  | 4:F:2516:ASP:OD1 | 2.43                     | 0.49              |
| 5:G:24:UNK:HG3    | 5:G:103:UNK:HA   | 1.95                     | 0.49              |
| 2:4:545:UNK:HG3   | 4:F:1395:LYS:HZ3 | 1.77                     | 0.49              |
| 3:A:1509:UNK:O    | 3:A:1525:UNK:N   | 2.45                     | 0.49              |
| 4:B:1445:ILE:HG13 | 4:B:1449:TRP:CZ3 | 2.47                     | 0.49              |
| 4:B:2379:LEU:O    | 4:B:2384:THR:OG1 | 2.30                     | 0.49              |
| 4:B:2512:ASP:OD1  | 4:B:2512:ASP:N   | 2.44                     | 0.49              |
| 3:E:765:UNK:HG2   | 3:E:766:UNK:HG2  | 1.95                     | 0.49              |
| 4:F:2139:ALA:HA   | 4:F:2152:ARG:HA  | 1.94                     | 0.49              |
| 4:B:1619:TRP:HA   | 4:B:1622:ARG:NH1 | 2.22                     | 0.49              |
| 4:B:2408:ARG:O    | 4:B:2411:LYS:HG2 | 2.12                     | 0.49              |
| 4:F:2254:ARG:HG3  | 4:F:2261:LEU:HA  | 1.95                     | 0.49              |
| 4:F:2374:LYS:HB2  | 4:F:2537:ASN:HB3 | 1.95                     | 0.49              |
| 1:1:1610:UNK:HG1  | 1:1:1709:UNK:HB1 | 1.95                     | 0.49              |
| 3:A:894:UNK:HA    | 3:A:937:UNK:HG1  | 1.94                     | 0.49              |
| 3:A:1509:UNK:HB1  | 3:A:1525:UNK:HB2 | 1.94                     | 0.49              |
| 4:B:1725:GLN:O    | 4:B:1729:GLN:HG2 | 2.13                     | 0.49              |
| 3:E:727:UNK:HG2   | 3:E:766:UNK:HG1  | 1.93                     | 0.49              |
| 4:F:1702:LYS:HG3  | 4:F:1706:LYS:HE3 | 1.95                     | 0.49              |
| 1:1:304:UNK:HB2   | 2:2:71:UNK:HB1   | 1.95                     | 0.49              |
| 4:B:1618:ILE:HA   | 4:B:1621:GLU:OE1 | 2.13                     | 0.49              |
| 4:F:1910:TRP:HZ2  | 4:F:1956:LEU:HB3 | 1.77                     | 0.49              |
| 6:H:17:THR:HB     | 6:H:27:TRP:HE1   | 1.77                     | 0.49              |
| 2:2:80:UNK:O      | 2:2:83:UNK:HG2   | 2.13                     | 0.49              |
| 1:3:1206:UNK:O    | 1:3:1210:UNK:HB1 | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4:181:UNK:O     | 2:4:184:UNK:HB2   | 2.13                     | 0.49              |
| 2:4:243:UNK:O     | 2:4:246:UNK:HG3   | 2.13                     | 0.49              |
| 3:A:882:UNK:HB1   | 3:A:885:UNK:HB1   | 1.95                     | 0.49              |
| 4:B:2074:TYR:HE2  | 4:B:2110:ARG:HB3  | 1.78                     | 0.49              |
| 4:B:2374:LYS:HB2  | 4:B:2537:ASN:HB3  | 1.95                     | 0.49              |
| 5:C:77:UNK:HA     | 5:C:96:UNK:HG3    | 1.93                     | 0.49              |
| 6:D:54:ARG:HD2    | 6:D:323:SER:HB2   | 1.94                     | 0.49              |
| 3:E:827:UNK:HG1   | 3:E:875:UNK:HG1   | 1.94                     | 0.49              |
| 4:F:1425:GLN:OE1  | 4:F:1426:PRO:HD2  | 2.13                     | 0.49              |
| 2:2:181:UNK:HA    | 2:2:184:UNK:HG2   | 1.93                     | 0.49              |
| 2:4:67:UNK:O      | 2:4:70:UNK:HB2    | 2.13                     | 0.49              |
| 2:4:545:UNK:O     | 2:4:548:UNK:HB2   | 2.13                     | 0.49              |
| 4:B:1581:GLU:HB2  | 4:B:1585:ARG:HB2  | 1.95                     | 0.49              |
| 6:D:242:GLN:OE1   | 6:D:270:ARG:N     | 2.46                     | 0.49              |
| 3:E:842:UNK:HG2   | 3:E:843:UNK:HG2   | 1.95                     | 0.49              |
| 4:F:1417:ILE:HG22 | 4:F:1429:ALA:HB1  | 1.95                     | 0.49              |
| 1:3:1103:UNK:HA   | 1:3:1304:UNK:HG1  | 1.95                     | 0.48              |
| 2:4:126:UNK:HB1   | 2:4:169:UNK:HB2   | 1.94                     | 0.48              |
| 2:4:232:UNK:C     | 2:4:234:UNK:N     | 2.76                     | 0.48              |
| 3:A:842:UNK:HG2   | 3:A:843:UNK:HG2   | 1.95                     | 0.48              |
| 4:B:1591:VAL:HG13 | 4:B:1636:ILE:HD11 | 1.93                     | 0.48              |
| 4:B:2133:CYS:SG   | 4:B:2136:LEU:HD11 | 2.53                     | 0.48              |
| 6:H:167:PRO:HG3   | 6:H:197:TRP:CZ2   | 2.45                     | 0.48              |
| 1:1:1113:UNK:HG1  | 1:1:1311:UNK:HB1  | 1.95                     | 0.48              |
| 2:4:45:UNK:O      | 2:4:49:UNK:HG2    | 2.13                     | 0.48              |
| 3:A:639:UNK:O     | 3:A:642:UNK:HB2   | 2.13                     | 0.48              |
| 4:B:1605:TYR:O    | 4:B:1612:ARG:NH1  | 2.46                     | 0.48              |
| 4:B:1631:GLU:OE2  | 4:B:1665:ARG:NH2  | 2.46                     | 0.48              |
| 4:F:1426:PRO:HG2  | 4:F:1427:GLU:CD   | 2.39                     | 0.48              |
| 2:2:45:UNK:O      | 2:2:49:UNK:HG2    | 2.13                     | 0.48              |
| 5:C:24:UNK:HG3    | 5:C:103:UNK:HA    | 1.94                     | 0.48              |
| 3:E:882:UNK:HB1   | 3:E:885:UNK:HB1   | 1.94                     | 0.48              |
| 4:F:1482:ARG:HA   | 4:F:1485:GLU:HG2  | 1.94                     | 0.48              |
| 4:F:2332:TYR:CZ   | 4:F:2507:LYS:HE2  | 2.49                     | 0.48              |
| 1:1:1018:UNK:O    | 1:1:1022:UNK:HB2  | 2.13                     | 0.48              |
| 1:3:1610:UNK:HG1  | 1:3:1709:UNK:HB1  | 1.94                     | 0.48              |
| 2:4:165:UNK:O     | 2:4:168:UNK:HB2   | 2.13                     | 0.48              |
| 3:A:916:UNK:HB1   | 3:A:931:UNK:HG2   | 1.96                     | 0.48              |
| 4:B:1603:ILE:O    | 4:B:1607:LEU:HB2  | 2.14                     | 0.48              |
| 4:F:2047:MET:O    | 4:F:2051:LEU:HB2  | 2.13                     | 0.48              |
| 1:1:1805:UNK:HG1  | 1:1:2003:UNK:HG1  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:160:UNK:HG1   | 2:2:197:UNK:HB2   | 1.94                     | 0.48              |
| 2:2:232:UNK:C     | 2:2:234:UNK:N     | 2.76                     | 0.48              |
| 1:3:103:UNK:HA    | 1:3:106:UNK:HB1   | 1.95                     | 0.48              |
| 2:4:310:UNK:HB2   | 2:4:404:UNK:HB2   | 1.95                     | 0.48              |
| 4:B:2047:MET:O    | 4:B:2051:LEU:HB2  | 2.13                     | 0.48              |
| 4:F:1725:GLN:O    | 4:F:1729:GLN:HG2  | 2.13                     | 0.48              |
| 4:F:2344:LEU:HD13 | 4:F:2353:ILE:HD11 | 1.96                     | 0.48              |
| 1:1:120:UNK:O     | 1:1:124:UNK:N     | 2.46                     | 0.48              |
| 2:4:80:UNK:O      | 2:4:83:UNK:HG2    | 2.14                     | 0.48              |
| 2:4:556:UNK:C     | 4:F:2257:LYS:HE2  | 2.44                     | 0.48              |
| 3:A:109:UNK:HB2   | 3:A:111:UNK:HG2   | 1.95                     | 0.48              |
| 4:B:2322:ARG:O    | 4:B:2326:VAL:HG23 | 2.13                     | 0.48              |
| 4:B:2344:LEU:HD13 | 4:B:2353:ILE:HD11 | 1.96                     | 0.48              |
| 4:B:2547:PRO:HD2  | 4:B:2548:PHE:CE2  | 2.49                     | 0.48              |
| 5:G:22:UNK:HB2    | 5:G:50:UNK:HG2    | 1.95                     | 0.48              |
| 1:1:206:UNK:O     | 1:1:209:UNK:HG3   | 2.13                     | 0.48              |
| 3:A:841:UNK:O     | 3:A:843:UNK:N     | 2.46                     | 0.48              |
| 4:B:1778:ALA:HA   | 4:B:1781:GLU:HG2  | 1.96                     | 0.48              |
| 4:B:2060:ARG:NH2  | 4:B:2061:GLY:O    | 2.31                     | 0.48              |
| 4:B:2415:MET:O    | 4:B:2419:GLU:HG3  | 2.14                     | 0.48              |
| 6:D:20:TYR:HB2    | 6:D:313:LYS:HB3   | 1.96                     | 0.48              |
| 3:E:916:UNK:HB1   | 3:E:931:UNK:HG2   | 1.96                     | 0.48              |
| 4:F:2133:CYS:SG   | 4:F:2136:LEU:HD11 | 2.53                     | 0.48              |
| 4:F:2547:PRO:HD2  | 4:F:2548:PHE:CE2  | 2.49                     | 0.48              |
| 1:1:1206:UNK:O    | 1:1:1210:UNK:HB1  | 2.13                     | 0.48              |
| 1:1:2113:UNK:HA   | 1:1:2116:UNK:HG3  | 1.96                     | 0.48              |
| 1:3:425:UNK:O     | 1:3:429:UNK:N     | 2.47                     | 0.48              |
| 2:4:174:UNK:HG1   | 2:4:211:UNK:HG2   | 1.95                     | 0.48              |
| 2:4:549:UNK:O     | 2:4:552:UNK:HG3   | 2.14                     | 0.48              |
| 4:B:2245:THR:HG22 | 4:B:2345:MET:HE2  | 1.96                     | 0.48              |
| 5:C:22:UNK:HB2    | 5:C:50:UNK:HG2    | 1.96                     | 0.48              |
| 3:E:808:UNK:O     | 3:E:812:UNK:N     | 2.47                     | 0.48              |
| 4:F:1414:GLU:HA   | 4:F:1417:ILE:HD11 | 1.96                     | 0.48              |
| 4:F:1603:ILE:O    | 4:F:1607:LEU:HB2  | 2.13                     | 0.48              |
| 4:F:1618:ILE:HA   | 4:F:1621:GLU:OE1  | 2.13                     | 0.48              |
| 4:F:2415:MET:O    | 4:F:2419:GLU:HG3  | 2.14                     | 0.48              |
| 2:2:67:UNK:O      | 2:2:70:UNK:HB2    | 2.14                     | 0.48              |
| 1:3:44:UNK:O      | 1:3:47:UNK:HB1    | 2.14                     | 0.48              |
| 3:A:590:UNK:HA    | 3:A:593:UNK:HB1   | 1.96                     | 0.48              |
| 4:F:2172:LEU:HB3  | 4:F:2184:PHE:O    | 2.13                     | 0.48              |
| 1:1:103:UNK:HA    | 1:1:106:UNK:HB1   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1103:UNK:HA   | 1:1:1304:UNK:HG1  | 1.96                     | 0.48              |
| 2:2:243:UNK:O     | 2:2:246:UNK:HG3   | 2.14                     | 0.48              |
| 1:3:206:UNK:O     | 1:3:209:UNK:HG3   | 2.14                     | 0.48              |
| 4:B:2172:LEU:HB3  | 4:B:2184:PHE:O    | 2.13                     | 0.48              |
| 6:D:269:SER:O     | 6:D:271:GLY:N     | 2.47                     | 0.48              |
| 3:E:841:UNK:O     | 3:E:843:UNK:N     | 2.46                     | 0.48              |
| 4:F:2222:ILE:HD11 | 4:F:2330:VAL:HG21 | 1.96                     | 0.48              |
| 1:1:425:UNK:O     | 1:1:429:UNK:N     | 2.47                     | 0.47              |
| 1:3:1:UNK:HG2     | 4:B:1594:HIS:CG   | 2.48                     | 0.47              |
| 4:B:1482:ARG:HA   | 4:B:1485:GLU:HG2  | 1.94                     | 0.47              |
| 4:B:1797:ASN:HB3  | 4:B:1884:ALA:HB2  | 1.95                     | 0.47              |
| 4:B:2031:LEU:HD23 | 4:B:2051:LEU:HD11 | 1.96                     | 0.47              |
| 3:E:109:UNK:HB2   | 3:E:111:UNK:HG2   | 1.95                     | 0.47              |
| 4:F:2074:TYR:HE2  | 4:F:2110:ARG:HB3  | 1.77                     | 0.47              |
| 4:F:2322:ARG:O    | 4:F:2326:VAL:HG23 | 2.13                     | 0.47              |
| 1:1:1:UNK:HG2     | 4:F:1594:HIS:CG   | 2.49                     | 0.47              |
| 2:2:165:UNK:O     | 2:2:168:UNK:HB2   | 2.13                     | 0.47              |
| 2:2:407:UNK:HG3   | 2:2:408:UNK:HB2   | 1.95                     | 0.47              |
| 3:A:604:UNK:HA    | 3:A:607:UNK:HB2   | 1.96                     | 0.47              |
| 4:B:2332:TYR:CZ   | 4:B:2507:LYS:HE2  | 2.49                     | 0.47              |
| 4:F:1529:MET:HE3  | 4:F:1550:LEU:HG   | 1.96                     | 0.47              |
| 2:2:181:UNK:O     | 2:2:184:UNK:HB2   | 2.13                     | 0.47              |
| 1:3:135:UNK:HB2   | 1:3:139:UNK:HG1   | 1.95                     | 0.47              |
| 1:3:1113:UNK:HG1  | 1:3:1311:UNK:HB1  | 1.95                     | 0.47              |
| 2:4:24:UNK:O      | 2:4:28:UNK:HB2    | 2.14                     | 0.47              |
| 3:A:581:UNK:O     | 3:A:585:UNK:HB2   | 2.14                     | 0.47              |
| 3:A:808:UNK:O     | 3:A:812:UNK:N     | 2.47                     | 0.47              |
| 4:F:1778:ALA:HA   | 4:F:1781:GLU:HG2  | 1.96                     | 0.47              |
| 4:F:2536:GLU:O    | 4:F:2540:GLN:NE2  | 2.47                     | 0.47              |
| 6:H:54:ARG:HD2    | 6:H:323:SER:HB2   | 1.95                     | 0.47              |
| 2:2:24:UNK:O      | 2:2:28:UNK:HB2    | 2.14                     | 0.47              |
| 2:4:407:UNK:HG3   | 2:4:408:UNK:HB2   | 1.97                     | 0.47              |
| 4:B:1529:MET:HE3  | 4:B:1550:LEU:HG   | 1.96                     | 0.47              |
| 4:B:2254:ARG:HG3  | 4:B:2261:LEU:HA   | 1.95                     | 0.47              |
| 2:2:556:UNK:C     | 4:B:2257:LYS:HE2  | 2.45                     | 0.47              |
| 1:3:1018:UNK:O    | 1:3:1022:UNK:HB2  | 2.14                     | 0.47              |
| 1:3:2011:UNK:HG3  | 1:3:2106:UNK:HG2  | 1.97                     | 0.47              |
| 4:B:2222:ILE:HD11 | 4:B:2330:VAL:HG21 | 1.96                     | 0.47              |
| 4:B:2521:VAL:HB   | 4:B:2522:PRO:HD3  | 1.96                     | 0.47              |
| 6:D:94:HIS:CD2    | 6:D:140:GLN:HE21  | 2.33                     | 0.47              |
| 6:H:262:SER:HA    | 6:H:270:ARG:NH1   | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4:110:UNK:O     | 2:4:114:UNK:HG2   | 2.15                     | 0.47              |
| 3:A:1330:UNK:HB1  | 3:A:1708:UNK:HG2  | 1.97                     | 0.47              |
| 4:B:1794:ALA:HB1  | 4:B:1888:PHE:CD2  | 2.50                     | 0.47              |
| 4:B:2172:LEU:HD23 | 4:B:2184:PHE:HB2  | 1.95                     | 0.47              |
| 4:F:1797:ASN:HB3  | 4:F:1884:ALA:HB2  | 1.95                     | 0.47              |
| 4:F:2140:VAL:HB   | 4:F:2143:THR:HG21 | 1.95                     | 0.47              |
| 6:H:269:SER:O     | 6:H:271:GLY:N     | 2.47                     | 0.47              |
| 1:1:135:UNK:HB2   | 1:1:139:UNK:HG1   | 1.95                     | 0.47              |
| 2:2:310:UNK:HB2   | 2:2:404:UNK:HB2   | 1.95                     | 0.47              |
| 2:2:545:UNK:O     | 2:2:548:UNK:HB2   | 2.13                     | 0.47              |
| 1:3:1:UNK:H       | 1:3:5:UNK:HB2     | 1.80                     | 0.47              |
| 2:4:533:UNK:O     | 2:4:537:UNK:HB2   | 2.15                     | 0.47              |
| 4:B:2140:VAL:HB   | 4:B:2143:THR:HG21 | 1.96                     | 0.47              |
| 3:E:639:UNK:O     | 3:E:642:UNK:HB2   | 2.13                     | 0.47              |
| 4:F:1521:TRP:HZ2  | 4:F:1642:LEU:HG   | 1.80                     | 0.47              |
| 4:F:1651:ARG:HA   | 4:F:1654:LEU:HD12 | 1.97                     | 0.47              |
| 4:F:2162:VAL:HA   | 4:F:2170:ARG:HA   | 1.97                     | 0.47              |
| 4:F:2172:LEU:HD23 | 4:F:2184:PHE:HB2  | 1.95                     | 0.47              |
| 4:F:2376:PRO:HD3  | 4:F:2531:GLN:NE2  | 2.30                     | 0.47              |
| 4:B:1426:PRO:HG2  | 4:B:1427:GLU:CD   | 2.39                     | 0.47              |
| 4:F:2521:VAL:HB   | 4:F:2522:PRO:HD3  | 1.96                     | 0.47              |
| 5:G:27:UNK:HB1    | 5:G:38:UNK:HG2    | 1.97                     | 0.47              |
| 6:H:94:HIS:CD2    | 6:H:140:GLN:HE21  | 2.33                     | 0.47              |
| 1:1:2011:UNK:HG3  | 1:1:2106:UNK:HG2  | 1.97                     | 0.47              |
| 4:B:1906:VAL:HG11 | 4:B:1935:TRP:HH2  | 1.80                     | 0.47              |
| 4:B:2162:VAL:HA   | 4:B:2170:ARG:HA   | 1.96                     | 0.47              |
| 4:B:2520:ASP:OD2  | 4:B:2522:PRO:HD2  | 2.15                     | 0.47              |
| 6:D:262:SER:HA    | 6:D:270:ARG:NH1   | 2.30                     | 0.47              |
| 4:F:2031:LEU:HD23 | 4:F:2051:LEU:HD11 | 1.95                     | 0.47              |
| 4:F:2428:ASN:HB3  | 4:F:2493:LEU:HD13 | 1.97                     | 0.47              |
| 1:1:44:UNK:O      | 1:1:47:UNK:HB1    | 2.14                     | 0.47              |
| 2:2:174:UNK:HG1   | 2:2:211:UNK:HG2   | 1.95                     | 0.47              |
| 1:3:24:UNK:HA     | 1:3:27:UNK:HG2    | 1.97                     | 0.47              |
| 1:3:141:UNK:C     | 1:3:143:UNK:HG2   | 2.45                     | 0.47              |
| 1:3:1507:UNK:HA   | 1:3:1510:UNK:HB1  | 1.97                     | 0.47              |
| 2:4:308:UNK:O     | 2:4:310:UNK:N     | 2.48                     | 0.47              |
| 3:A:1508:UNK:HB2  | 3:A:1552:UNK:HB2  | 1.96                     | 0.47              |
| 3:A:1715:UNK:HG3  | 3:A:1726:UNK:HG3  | 1.97                     | 0.47              |
| 4:B:2379:LEU:HD13 | 4:B:2379:LEU:HA   | 1.70                     | 0.47              |
| 4:B:2536:GLU:O    | 4:B:2540:GLN:NE2  | 2.47                     | 0.47              |
| 3:E:567:UNK:O     | 3:E:569:UNK:N     | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1605:UNK:HB2  | 3:E:1635:UNK:HG1  | 1.96                     | 0.47              |
| 4:F:1481:MET:HE3  | 4:F:1493:LEU:HD11 | 1.97                     | 0.47              |
| 4:F:1619:TRP:HA   | 4:F:1622:ARG:NH1  | 2.21                     | 0.47              |
| 4:F:1794:ALA:HB1  | 4:F:1888:PHE:CD2  | 2.50                     | 0.47              |
| 4:F:2379:LEU:O    | 4:F:2384:THR:OG1  | 2.31                     | 0.47              |
| 4:F:2520:ASP:OD2  | 4:F:2522:PRO:HD2  | 2.15                     | 0.47              |
| 1:1:141:UNK:C     | 1:1:143:UNK:HG2   | 2.45                     | 0.46              |
| 1:1:2001:UNK:HG3  | 1:1:2200:UNK:HG3  | 1.98                     | 0.46              |
| 2:4:142:UNK:HG3   | 2:4:143:UNK:HG2   | 1.98                     | 0.46              |
| 3:A:765:UNK:HG2   | 3:A:766:UNK:HG2   | 1.96                     | 0.46              |
| 4:B:1414:GLU:HA   | 4:B:1417:ILE:HD11 | 1.97                     | 0.46              |
| 4:B:1472:ASP:CG   | 4:B:1503:LEU:HD13 | 2.40                     | 0.46              |
| 4:B:1481:MET:HE3  | 4:B:1493:LEU:HD11 | 1.97                     | 0.46              |
| 4:B:1899:ASN:HB2  | 4:B:1903:THR:OG1  | 2.15                     | 0.46              |
| 3:E:604:UNK:HA    | 3:E:607:UNK:HB2   | 1.97                     | 0.46              |
| 4:F:1906:VAL:HG11 | 4:F:1935:TRP:HH2  | 1.80                     | 0.46              |
| 6:H:20:TYR:HB2    | 6:H:313:LYS:HB3   | 1.96                     | 0.46              |
| 6:H:222:TYR:O     | 6:H:239:SER:OG    | 2.27                     | 0.46              |
| 1:1:24:UNK:HA     | 1:1:27:UNK:HG2    | 1.96                     | 0.46              |
| 1:3:88:UNK:HA     | 1:3:91:UNK:CB     | 2.46                     | 0.46              |
| 3:A:567:UNK:O     | 3:A:569:UNK:N     | 2.48                     | 0.46              |
| 4:B:1425:GLN:OE1  | 4:B:1426:PRO:HD2  | 2.13                     | 0.46              |
| 3:E:590:UNK:HA    | 3:E:593:UNK:HB1   | 1.96                     | 0.46              |
| 3:E:1104:UNK:O    | 3:E:1108:UNK:HB2  | 2.15                     | 0.46              |
| 3:E:1508:UNK:HB2  | 3:E:1552:UNK:HB2  | 1.96                     | 0.46              |
| 6:H:132:ASN:H     | 6:H:147:ASP:HA    | 1.81                     | 0.46              |
| 6:H:297:TRP:CZ3   | 6:H:304:ILE:HG12  | 2.50                     | 0.46              |
| 1:3:1407:UNK:HG2  | 1:3:1509:UNK:HG2  | 1.97                     | 0.46              |
| 1:3:2001:UNK:HG3  | 1:3:2200:UNK:HG3  | 1.97                     | 0.46              |
| 4:B:1605:TYR:CZ   | 4:B:1612:ARG:HD2  | 2.51                     | 0.46              |
| 4:B:1651:ARG:HA   | 4:B:1654:LEU:HD12 | 1.98                     | 0.46              |
| 4:B:2290:ALA:O    | 4:B:2294:THR:OG1  | 2.19                     | 0.46              |
| 5:C:27:UNK:HB1    | 5:C:38:UNK:HG2    | 1.98                     | 0.46              |
| 6:D:65:ILE:HG13   | 6:D:88:ILE:HD13   | 1.98                     | 0.46              |
| 3:E:1328:UNK:HB2  | 3:E:1706:UNK:HG1  | 1.97                     | 0.46              |
| 3:E:1330:UNK:HB1  | 3:E:1708:UNK:HG2  | 1.97                     | 0.46              |
| 1:1:42:UNK:HB2    | 4:F:1611:ARG:NH1  | 2.30                     | 0.46              |
| 1:3:7:UNK:HA      | 1:3:10:UNK:HB2    | 1.97                     | 0.46              |
| 1:3:435:UNK:HG1   | 1:3:447:UNK:HG1   | 1.98                     | 0.46              |
| 2:4:158:UNK:HG3   | 2:4:162:UNK:HB1   | 1.96                     | 0.46              |
| 3:A:1104:UNK:O    | 3:A:1108:UNK:HB2  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:88:ILE:HA     | 6:D:104:GLY:HA2   | 1.97                     | 0.46              |
| 6:D:198:ASN:ND2   | 6:D:213:LYS:HB2   | 2.31                     | 0.46              |
| 4:F:1437:MET:HE3  | 4:F:1446:GLN:NE2  | 2.30                     | 0.46              |
| 4:F:1472:ASP:CG   | 4:F:1503:LEU:HD13 | 2.41                     | 0.46              |
| 1:1:88:UNK:HA     | 1:1:91:UNK:CB     | 2.45                     | 0.46              |
| 3:A:840:UNK:O     | 3:A:842:UNK:HG3   | 2.16                     | 0.46              |
| 3:E:840:UNK:O     | 3:E:842:UNK:HG3   | 2.16                     | 0.46              |
| 4:F:2245:THR:HG22 | 4:F:2345:MET:HE2  | 1.97                     | 0.46              |
| 2:2:533:UNK:O     | 2:2:537:UNK:HB2   | 2.14                     | 0.46              |
| 1:3:42:UNK:HB2    | 4:B:1611:ARG:NH1  | 2.30                     | 0.46              |
| 1:3:440:UNK:HB1   | 1:3:443:UNK:HB2   | 1.98                     | 0.46              |
| 1:3:612:UNK:O     | 1:3:615:UNK:HB1   | 2.15                     | 0.46              |
| 6:D:297:TRP:CZ3   | 6:D:304:ILE:HG12  | 2.50                     | 0.46              |
| 4:F:1665:ARG:HH11 | 4:F:1668:LEU:HD22 | 1.81                     | 0.46              |
| 6:H:228:PHE:CE1   | 6:H:235:LEU:HB2   | 2.51                     | 0.46              |
| 1:1:151:UNK:O     | 1:1:155:UNK:HG3   | 2.15                     | 0.46              |
| 2:2:86:UNK:O      | 2:2:90:UNK:HG2    | 2.15                     | 0.46              |
| 1:3:142:UNK:O     | 1:3:145:UNK:N     | 2.49                     | 0.46              |
| 1:3:2113:UNK:HA   | 1:3:2116:UNK:HG3  | 1.96                     | 0.46              |
| 2:4:86:UNK:O      | 2:4:90:UNK:HG2    | 2.15                     | 0.46              |
| 4:F:1575:LEU:HA   | 4:F:1575:LEU:HD23 | 1.77                     | 0.46              |
| 4:F:1899:ASN:HB2  | 4:F:1903:THR:OG1  | 2.15                     | 0.46              |
| 1:1:82:UNK:O      | 1:1:85:UNK:HB2    | 2.16                     | 0.46              |
| 1:3:82:UNK:O      | 1:3:85:UNK:HB2    | 2.16                     | 0.46              |
| 1:3:151:UNK:O     | 1:3:155:UNK:HG3   | 2.16                     | 0.46              |
| 3:A:1328:UNK:HB2  | 3:A:1706:UNK:HG1  | 1.97                     | 0.46              |
| 4:B:1521:TRP:HZ2  | 4:B:1642:LEU:HG   | 1.80                     | 0.46              |
| 4:B:2254:ARG:NH1  | 4:B:2298:ASP:OD2  | 2.49                     | 0.46              |
| 4:B:2428:ASN:HB3  | 4:B:2493:LEU:HD13 | 1.97                     | 0.46              |
| 6:D:132:ASN:H     | 6:D:147:ASP:HA    | 1.81                     | 0.46              |
| 3:E:854:UNK:HG3   | 3:E:861:UNK:HG3   | 1.98                     | 0.46              |
| 6:H:88:ILE:HA     | 6:H:104:GLY:HA2   | 1.97                     | 0.46              |
| 1:1:7:UNK:HA      | 1:1:10:UNK:HB2    | 1.97                     | 0.46              |
| 1:1:320:UNK:O     | 1:1:323:UNK:N     | 2.49                     | 0.46              |
| 1:1:612:UNK:O     | 1:1:615:UNK:HB1   | 2.15                     | 0.46              |
| 1:3:1007:UNK:O    | 1:3:1011:UNK:HB2  | 2.16                     | 0.46              |
| 3:A:1605:UNK:HB2  | 3:A:1635:UNK:HG1  | 1.96                     | 0.46              |
| 4:B:2376:PRO:HD3  | 4:B:2531:GLN:NE2  | 2.31                     | 0.46              |
| 3:E:576:UNK:O     | 3:E:579:UNK:HG2   | 2.16                     | 0.46              |
| 4:F:2285:GLU:HB2  | 6:H:272:TRP:CH2   | 2.51                     | 0.46              |
| 1:1:210:UNK:C     | 1:1:212:UNK:N     | 2.79                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:142:UNK:HG3   | 2:2:143:UNK:HG2   | 1.97                     | 0.46              |
| 1:3:210:UNK:C     | 1:3:212:UNK:N     | 2.79                     | 0.46              |
| 1:3:448:UNK:HA    | 1:3:451:UNK:HB1   | 1.98                     | 0.46              |
| 1:3:1212:UNK:O    | 1:3:1216:UNK:HB2  | 2.16                     | 0.46              |
| 2:4:532:UNK:O     | 2:4:535:UNK:HB2   | 2.16                     | 0.46              |
| 3:E:1641:UNK:O    | 3:E:1643:UNK:N    | 2.49                     | 0.46              |
| 3:E:1715:UNK:HG3  | 3:E:1726:UNK:HG3  | 1.97                     | 0.46              |
| 4:F:2254:ARG:NH1  | 4:F:2298:ASP:OD2  | 2.49                     | 0.46              |
| 1:1:448:UNK:HA    | 1:1:451:UNK:HB1   | 1.98                     | 0.45              |
| 2:2:110:UNK:O     | 2:2:114:UNK:HG2   | 2.16                     | 0.45              |
| 2:2:158:UNK:HG3   | 2:2:162:UNK:HB1   | 1.98                     | 0.45              |
| 2:2:308:UNK:O     | 2:2:310:UNK:N     | 2.48                     | 0.45              |
| 3:A:1136:UNK:HG3  | 3:A:1144:UNK:HG2  | 1.98                     | 0.45              |
| 3:A:1332:UNK:HB2  | 3:A:1378:UNK:HB1  | 1.98                     | 0.45              |
| 4:F:2530:LYS:HE3  | 4:F:2530:LYS:HA   | 1.98                     | 0.45              |
| 6:H:198:ASN:ND2   | 6:H:213:LYS:HB2   | 2.31                     | 0.45              |
| 1:1:1212:UNK:O    | 1:1:1216:UNK:HB2  | 2.16                     | 0.45              |
| 1:1:1407:UNK:HG2  | 1:1:1509:UNK:HG2  | 1.97                     | 0.45              |
| 1:3:2109:UNK:O    | 1:3:2113:UNK:HB1  | 2.16                     | 0.45              |
| 3:A:719:UNK:O     | 3:A:723:UNK:HB1   | 2.16                     | 0.45              |
| 4:B:2039:PHE:HB3  | 7:C:999:RAP:H382  | 1.98                     | 0.45              |
| 3:E:204:UNK:HA    | 3:E:526:UNK:HG2   | 1.99                     | 0.45              |
| 4:F:2147:ASN:O    | 4:F:2148:GLN:NE2  | 2.32                     | 0.45              |
| 1:1:9:UNK:O       | 1:1:12:UNK:HG3    | 2.17                     | 0.45              |
| 1:3:118:UNK:C     | 1:3:120:UNK:N     | 2.79                     | 0.45              |
| 4:B:2162:VAL:HG22 | 4:B:2170:ARG:HG3  | 1.98                     | 0.45              |
| 4:B:2530:LYS:HA   | 4:B:2530:LYS:HE3  | 1.98                     | 0.45              |
| 3:E:719:UNK:O     | 3:E:723:UNK:HB1   | 2.16                     | 0.45              |
| 1:1:450:UNK:HA    | 1:1:453:UNK:HG3   | 1.99                     | 0.45              |
| 1:3:211:UNK:HB1   | 1:3:302:UNK:HB1   | 1.99                     | 0.45              |
| 4:B:1896:ARG:NH2  | 4:B:1931:GLN:HG3  | 2.31                     | 0.45              |
| 4:B:2285:GLU:HB2  | 6:D:272:TRP:CH2   | 2.51                     | 0.45              |
| 2:2:532:UNK:O     | 2:2:535:UNK:HB2   | 2.16                     | 0.45              |
| 3:A:714:UNK:HG1   | 3:A:738:UNK:HG1   | 1.98                     | 0.45              |
| 3:A:1641:UNK:O    | 3:A:1643:UNK:N    | 2.50                     | 0.45              |
| 4:B:2278:LEU:HB3  | 4:B:2282:GLN:HB2  | 1.97                     | 0.45              |
| 3:E:232:UNK:HB2   | 3:E:601:UNK:HG2   | 1.98                     | 0.45              |
| 3:E:714:UNK:HG1   | 3:E:738:UNK:HG1   | 1.99                     | 0.45              |
| 3:E:988:UNK:HB1   | 3:E:1102:UNK:HG1  | 1.99                     | 0.45              |
| 4:F:1433:LEU:HA   | 4:F:1433:LEU:HD12 | 1.66                     | 0.45              |
| 4:F:2278:LEU:HB3  | 4:F:2282:GLN:HB2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:2279:THR:N    | 4:F:2282:GLN:OE1  | 2.40                     | 0.45              |
| 6:H:65:ILE:HG13   | 6:H:88:ILE:HD13   | 1.97                     | 0.45              |
| 1:1:1:UNK:H       | 1:1:5:UNK:HB2     | 1.81                     | 0.45              |
| 1:1:36:UNK:HG3    | 1:1:37:UNK:HG2    | 1.99                     | 0.45              |
| 1:1:66:UNK:O      | 1:1:70:UNK:N      | 2.50                     | 0.45              |
| 1:1:70:UNK:O      | 1:1:74:UNK:HB2    | 2.17                     | 0.45              |
| 1:1:2004:UNK:HG1  | 1:1:2200:UNK:HG1  | 1.99                     | 0.45              |
| 1:3:154:UNK:HG3   | 3:E:643:UNK:CB    | 2.41                     | 0.45              |
| 2:4:167:UNK:O     | 2:4:171:UNK:HG2   | 2.17                     | 0.45              |
| 3:A:232:UNK:HB2   | 3:A:601:UNK:HG2   | 1.97                     | 0.45              |
| 4:B:1501:TRP:O    | 4:B:1504:VAL:HG22 | 2.17                     | 0.45              |
| 4:B:2519:LEU:HB3  | 4:B:2524:GLN:HB2  | 1.99                     | 0.45              |
| 6:D:289:SER:HB2   | 6:D:291:ASP:OD1   | 2.16                     | 0.45              |
| 4:F:2378:ARG:NH2  | 4:F:2545:TRP:O    | 2.50                     | 0.45              |
| 1:1:118:UNK:C     | 1:1:120:UNK:N     | 2.79                     | 0.45              |
| 1:1:142:UNK:O     | 1:1:145:UNK:N     | 2.50                     | 0.45              |
| 1:1:1507:UNK:HA   | 1:1:1510:UNK:HB1  | 1.97                     | 0.45              |
| 2:2:552:UNK:CG    | 4:B:2304:TRP:HZ2  | 2.26                     | 0.45              |
| 2:4:6:UNK:O       | 2:4:9:UNK:HB2     | 2.17                     | 0.45              |
| 3:A:204:UNK:HA    | 3:A:526:UNK:HG2   | 1.98                     | 0.45              |
| 3:A:748:UNK:O     | 3:A:752:UNK:HG2   | 2.17                     | 0.45              |
| 3:A:854:UNK:HG3   | 3:A:861:UNK:HG3   | 1.98                     | 0.45              |
| 4:B:1478:LEU:HD11 | 4:B:1508:THR:HG23 | 1.98                     | 0.45              |
| 5:C:26:UNK:O      | 5:C:39:UNK:N      | 2.50                     | 0.45              |
| 4:F:1478:LEU:HD11 | 4:F:1508:THR:HG23 | 1.99                     | 0.45              |
| 4:F:2017:ILE:HD13 | 4:F:2231:SER:HB3  | 1.99                     | 0.45              |
| 4:F:2512:ASP:OD1  | 4:F:2512:ASP:N    | 2.44                     | 0.45              |
| 2:2:302:UNK:O     | 2:2:306:UNK:HG2   | 2.17                     | 0.45              |
| 2:4:197:UNK:C     | 2:4:201:UNK:HG3   | 2.46                     | 0.45              |
| 3:A:225:UNK:HG3   | 3:A:237:UNK:HB2   | 1.98                     | 0.45              |
| 3:A:503:UNK:O     | 3:A:626:UNK:HB2   | 2.17                     | 0.45              |
| 3:A:639:UNK:O     | 3:A:643:UNK:HG3   | 2.17                     | 0.45              |
| 4:B:1427:GLU:O    | 4:B:1430:ALA:HB3  | 2.17                     | 0.45              |
| 4:B:1435:TYR:CG   | 4:B:2390:THR:HG21 | 2.51                     | 0.45              |
| 4:B:1665:ARG:HH11 | 4:B:1668:LEU:HD22 | 1.81                     | 0.45              |
| 4:B:1995:LEU:HD22 | 4:B:2010:MET:HE1  | 1.99                     | 0.45              |
| 3:E:1332:UNK:HB2  | 3:E:1378:UNK:HB1  | 1.98                     | 0.45              |
| 4:F:1416:LEU:HD23 | 4:F:1432:VAL:HG13 | 1.98                     | 0.45              |
| 1:1:123:UNK:O     | 1:1:126:UNK:HB2   | 2.17                     | 0.45              |
| 1:1:706:UNK:O     | 1:1:710:UNK:HB1   | 2.17                     | 0.45              |
| 2:2:197:UNK:C     | 2:2:201:UNK:HG3   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3:450:UNK:HA    | 1:3:453:UNK:HG3   | 1.99                     | 0.45              |
| 3:A:805:UNK:HG3   | 3:A:807:UNK:HB1   | 1.99                     | 0.45              |
| 4:B:1433:LEU:HD12 | 4:B:1433:LEU:HA   | 1.65                     | 0.45              |
| 4:B:1904:LEU:HD13 | 4:B:2417:VAL:HA   | 1.99                     | 0.45              |
| 6:D:228:PHE:CE1   | 6:D:235:LEU:HB2   | 2.52                     | 0.45              |
| 4:F:1501:TRP:O    | 4:F:1504:VAL:HG22 | 2.17                     | 0.45              |
| 4:F:2317:ARG:O    | 4:F:2321:THR:OG1  | 2.34                     | 0.45              |
| 6:H:188:VAL:HB    | 6:H:226:CYS:SG    | 2.57                     | 0.45              |
| 1:3:36:UNK:HG3    | 1:3:37:UNK:HG2    | 1.99                     | 0.45              |
| 1:3:123:UNK:O     | 1:3:126:UNK:HB2   | 2.16                     | 0.45              |
| 3:A:735:UNK:O     | 3:A:738:UNK:HB1   | 2.16                     | 0.45              |
| 4:B:1890:ARG:HE   | 4:B:1890:ARG:HB2  | 1.54                     | 0.45              |
| 4:F:1422:LYS:HE3  | 4:F:1422:LYS:HB2  | 1.68                     | 0.45              |
| 4:F:1605:TYR:HD2  | 4:F:1615:ILE:HD12 | 1.82                     | 0.45              |
| 4:F:1605:TYR:CZ   | 4:F:1612:ARG:HD2  | 2.51                     | 0.45              |
| 4:F:2541:CYS:SG   | 4:F:2542:TYR:N    | 2.89                     | 0.45              |
| 1:3:706:UNK:O     | 1:3:710:UNK:HB1   | 2.17                     | 0.44              |
| 2:4:78:UNK:HB1    | 3:E:634:UNK:HA    | 1.99                     | 0.44              |
| 4:B:1605:TYR:HD2  | 4:B:1615:ILE:HD12 | 1.82                     | 0.44              |
| 4:B:2411:LYS:HB2  | 4:B:2411:LYS:HE3  | 1.70                     | 0.44              |
| 6:D:28:GLN:HE21   | 6:D:33:ILE:HB     | 1.82                     | 0.44              |
| 6:D:188:VAL:HB    | 6:D:226:CYS:SG    | 2.57                     | 0.44              |
| 3:E:561:UNK:HA    | 3:E:569:UNK:HG3   | 1.99                     | 0.44              |
| 3:E:735:UNK:O     | 3:E:738:UNK:HB1   | 2.17                     | 0.44              |
| 4:F:1777:SER:O    | 4:F:1781:GLU:HG2  | 2.17                     | 0.44              |
| 1:1:319:UNK:O     | 1:1:324:UNK:HB2   | 2.18                     | 0.44              |
| 2:2:6:UNK:O       | 2:2:9:UNK:HB2     | 2.17                     | 0.44              |
| 1:3:48:UNK:HA     | 1:3:51:UNK:CG     | 2.47                     | 0.44              |
| 1:3:70:UNK:O      | 1:3:74:UNK:HB2    | 2.17                     | 0.44              |
| 1:3:713:UNK:HG1   | 1:3:909:UNK:HB1   | 1.99                     | 0.44              |
| 3:A:576:UNK:O     | 3:A:579:UNK:HG2   | 2.17                     | 0.44              |
| 3:A:1604:UNK:HG2  | 3:A:1612:UNK:HG2  | 1.99                     | 0.44              |
| 4:B:2545:TRP:HZ3  | 4:B:2547:PRO:HA   | 1.83                     | 0.44              |
| 3:E:225:UNK:HG3   | 3:E:237:UNK:HB2   | 1.99                     | 0.44              |
| 3:E:410:UNK:HG3   | 3:E:413:UNK:HB1   | 1.98                     | 0.44              |
| 3:E:805:UNK:HG3   | 3:E:807:UNK:HB1   | 1.99                     | 0.44              |
| 4:F:2039:PHE:HB3  | 7:G:999:RAP:H382  | 1.98                     | 0.44              |
| 4:F:2397:ARG:HH11 | 4:F:2397:ARG:HB2  | 1.82                     | 0.44              |
| 1:1:211:UNK:HB1   | 1:1:302:UNK:HB1   | 1.99                     | 0.44              |
| 1:1:1007:UNK:O    | 1:1:1011:UNK:HB2  | 2.16                     | 0.44              |
| 2:2:167:UNK:O     | 2:2:171:UNK:HG2   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1743:LEU:O    | 4:B:1747:MET:HG3  | 2.18                     | 0.44              |
| 4:B:2397:ARG:HA   | 4:B:2400:CYS:SG   | 2.58                     | 0.44              |
| 4:B:2513:PHE:HE2  | 4:B:2528:LEU:HG   | 1.82                     | 0.44              |
| 4:B:2541:CYS:SG   | 4:B:2542:TYR:N    | 2.90                     | 0.44              |
| 3:E:1604:UNK:HG2  | 3:E:1612:UNK:HG2  | 2.00                     | 0.44              |
| 4:F:1568:ARG:NH2  | 4:F:1600:GLU:OE2  | 2.51                     | 0.44              |
| 4:F:1743:LEU:O    | 4:F:1747:MET:HG3  | 2.18                     | 0.44              |
| 4:F:2051:LEU:HD12 | 4:F:2051:LEU:HA   | 1.79                     | 0.44              |
| 4:F:2513:PHE:HE2  | 4:F:2528:LEU:HG   | 1.82                     | 0.44              |
| 6:H:289:SER:HB2   | 6:H:291:ASP:OD1   | 2.16                     | 0.44              |
| 1:3:2303:UNK:O    | 1:3:2307:UNK:HB2  | 2.18                     | 0.44              |
| 3:A:410:UNK:HG3   | 3:A:413:UNK:HB1   | 1.98                     | 0.44              |
| 3:E:1136:UNK:HG3  | 3:E:1144:UNK:HG2  | 1.98                     | 0.44              |
| 4:F:1421:ASN:HD21 | 4:F:1452:LYS:HB3  | 1.83                     | 0.44              |
| 4:F:1453:LEU:HD22 | 4:F:1453:LEU:HA   | 1.81                     | 0.44              |
| 6:H:28:GLN:HE21   | 6:H:33:ILE:HB     | 1.82                     | 0.44              |
| 1:3:66:UNK:O      | 1:3:70:UNK:N      | 2.50                     | 0.44              |
| 1:3:320:UNK:O     | 1:3:323:UNK:N     | 2.51                     | 0.44              |
| 4:B:1530:GLU:HA   | 4:B:1550:LEU:HD11 | 2.00                     | 0.44              |
| 4:B:2404:MET:HB3  | 4:B:2521:VAL:HG13 | 2.00                     | 0.44              |
| 3:E:745:UNK:HG2   | 3:E:747:UNK:N     | 2.32                     | 0.44              |
| 4:F:1515:MET:H    | 4:F:1515:MET:HG3  | 1.60                     | 0.44              |
| 4:F:2404:MET:HB3  | 4:F:2521:VAL:HG13 | 2.00                     | 0.44              |
| 4:F:2543:ILE:HD12 | 4:F:2543:ILE:HA   | 1.76                     | 0.44              |
| 1:1:1216:UNK:HB1  | 1:1:1305:UNK:HG1  | 2.00                     | 0.44              |
| 1:1:2109:UNK:O    | 1:1:2113:UNK:HB1  | 2.17                     | 0.44              |
| 1:3:32:UNK:O      | 1:3:34:UNK:N      | 2.51                     | 0.44              |
| 1:3:52:UNK:HG1    | 1:3:90:UNK:HB2    | 2.00                     | 0.44              |
| 2:4:151:UNK:O     | 2:4:152:UNK:C     | 2.65                     | 0.44              |
| 4:B:1407:GLY:HA2  | 4:B:1408:PRO:HD3  | 1.81                     | 0.44              |
| 4:B:1560:ALA:O    | 4:B:1564:ILE:HG13 | 2.18                     | 0.44              |
| 4:B:2317:ARG:O    | 4:B:2321:THR:OG1  | 2.35                     | 0.44              |
| 3:E:639:UNK:O     | 3:E:643:UNK:HG3   | 2.18                     | 0.44              |
| 3:E:643:UNK:O     | 3:E:646:UNK:HB1   | 2.18                     | 0.44              |
| 3:A:1638:UNK:HG2  | 3:A:1707:UNK:HB1  | 2.00                     | 0.44              |
| 4:B:1422:LYS:HB2  | 4:B:1422:LYS:HE3  | 1.67                     | 0.44              |
| 4:F:1896:ARG:NH2  | 4:F:1931:GLN:HG3  | 2.31                     | 0.44              |
| 4:F:2519:LEU:HB3  | 4:F:2524:GLN:HB2  | 1.99                     | 0.44              |
| 1:1:706:UNK:HB1   | 1:1:902:UNK:HB1   | 2.00                     | 0.44              |
| 2:2:514:UNK:O     | 2:2:518:UNK:HB1   | 2.17                     | 0.44              |
| 1:3:8:UNK:O       | 1:3:12:UNK:HB1    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3:32:UNK:O      | 1:3:33:UNK:C      | 2.66                     | 0.44              |
| 1:3:1306:UNK:O    | 1:3:1310:UNK:HG2  | 2.18                     | 0.44              |
| 2:4:9:UNK:O       | 2:4:13:UNK:HB2    | 2.18                     | 0.44              |
| 2:4:514:UNK:O     | 2:4:518:UNK:HB1   | 2.17                     | 0.44              |
| 4:B:1972:LEU:HB3  | 4:B:1976:LEU:HD12 | 2.00                     | 0.44              |
| 4:B:2543:ILE:HA   | 4:B:2543:ILE:HD12 | 1.77                     | 0.44              |
| 4:F:1427:GLU:O    | 4:F:1430:ALA:HB3  | 2.17                     | 0.44              |
| 4:F:1904:LEU:HD13 | 4:F:2417:VAL:HA   | 1.99                     | 0.44              |
| 4:F:2545:TRP:HZ3  | 4:F:2547:PRO:HA   | 1.83                     | 0.44              |
| 1:1:1306:UNK:O    | 1:1:1310:UNK:HG2  | 2.18                     | 0.44              |
| 2:2:26:UNK:O      | 2:2:30:UNK:HG2    | 2.18                     | 0.44              |
| 1:3:4:UNK:O       | 1:3:7:UNK:HB1     | 2.17                     | 0.44              |
| 1:3:436:UNK:HA    | 1:3:444:UNK:HB2   | 2.00                     | 0.44              |
| 3:A:1362:UNK:HB1  | 3:A:1364:UNK:HG2  | 2.00                     | 0.44              |
| 3:E:503:UNK:O     | 3:E:626:UNK:HB2   | 2.18                     | 0.44              |
| 3:E:748:UNK:O     | 3:E:752:UNK:HG2   | 2.17                     | 0.44              |
| 3:E:1362:UNK:HB1  | 3:E:1364:UNK:HG2  | 1.99                     | 0.44              |
| 4:F:2397:ARG:HG2  | 4:F:2401:HIS:NE2  | 2.33                     | 0.44              |
| 1:1:48:UNK:HA     | 1:1:51:UNK:CG     | 2.47                     | 0.43              |
| 1:1:54:UNK:HA     | 1:1:57:UNK:HB2    | 1.99                     | 0.43              |
| 1:3:2004:UNK:HG1  | 1:3:2200:UNK:HG1  | 1.99                     | 0.43              |
| 2:4:302:UNK:O     | 2:4:306:UNK:HG2   | 2.18                     | 0.43              |
| 3:A:929:UNK:HB2   | 3:A:973:UNK:HB2   | 2.00                     | 0.43              |
| 3:A:1538:UNK:HB1  | 3:A:1540:UNK:HG3  | 2.00                     | 0.43              |
| 5:C:4:UNK:HG2     | 5:C:62:UNK:HG3    | 2.00                     | 0.43              |
| 6:D:271:GLY:HA3   | 6:D:290:SER:HB2   | 2.00                     | 0.43              |
| 3:E:803:UNK:HB1   | 3:E:1217:UNK:HG2  | 2.00                     | 0.43              |
| 4:F:1530:GLU:HA   | 4:F:1550:LEU:HD11 | 2.00                     | 0.43              |
| 4:F:1613:GLU:H    | 4:F:1613:GLU:HG3  | 1.48                     | 0.43              |
| 4:F:1995:LEU:HD22 | 4:F:2010:MET:HE1  | 1.99                     | 0.43              |
| 1:1:8:UNK:O       | 1:1:12:UNK:HB1    | 2.18                     | 0.43              |
| 1:1:306:UNK:O     | 1:1:310:UNK:HB2   | 2.18                     | 0.43              |
| 1:1:438:UNK:HB2   | 1:1:439:UNK:H     | 1.55                     | 0.43              |
| 1:1:440:UNK:HB1   | 1:1:443:UNK:HB2   | 1.99                     | 0.43              |
| 1:1:1313:UNK:HG1  | 1:1:1400:UNK:HB1  | 2.00                     | 0.43              |
| 1:3:9:UNK:O       | 1:3:12:UNK:HG3    | 2.17                     | 0.43              |
| 2:4:26:UNK:O      | 2:4:30:UNK:HG2    | 2.19                     | 0.43              |
| 3:A:643:UNK:O     | 3:A:646:UNK:HB1   | 2.18                     | 0.43              |
| 3:A:988:UNK:HB1   | 3:A:1102:UNK:HG1  | 1.99                     | 0.43              |
| 4:B:1977:THR:O    | 4:B:1980:SER:OG   | 2.27                     | 0.43              |
| 6:D:132:ASN:ND2   | 6:D:148:GLN:HG2   | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1310:UNK:CG   | 1:1:1512:UNK:HA   | 2.49                     | 0.43              |
| 2:2:9:UNK:O       | 2:2:13:UNK:HB2    | 2.18                     | 0.43              |
| 1:3:306:UNK:O     | 1:3:308:UNK:N     | 2.51                     | 0.43              |
| 3:A:561:UNK:HA    | 3:A:569:UNK:HG3   | 1.99                     | 0.43              |
| 4:B:1777:SER:O    | 4:B:1781:GLU:HG2  | 2.17                     | 0.43              |
| 4:B:2017:ILE:HD13 | 4:B:2231:SER:HB3  | 2.00                     | 0.43              |
| 4:F:1530:GLU:O    | 4:F:1533:THR:HB   | 2.19                     | 0.43              |
| 4:F:1972:LEU:HB3  | 4:F:1976:LEU:HD12 | 2.00                     | 0.43              |
| 4:F:2162:VAL:HG22 | 4:F:2170:ARG:HG3  | 2.00                     | 0.43              |
| 4:F:2299:LEU:O    | 4:F:2302:LEU:HG   | 2.19                     | 0.43              |
| 6:H:19:GLY:HA2    | 6:H:316:VAL:HG23  | 2.00                     | 0.43              |
| 1:1:4:UNK:O       | 1:1:5:UNK:C       | 2.67                     | 0.43              |
| 3:A:745:UNK:HG2   | 3:A:747:UNK:N     | 2.32                     | 0.43              |
| 4:B:1416:LEU:HD23 | 4:B:1432:VAL:HG13 | 2.00                     | 0.43              |
| 4:B:1530:GLU:O    | 4:B:1533:THR:HB   | 2.19                     | 0.43              |
| 4:B:2340:HIS:O    | 4:B:2343:ASN:N    | 2.47                     | 0.43              |
| 4:B:2378:ARG:NH2  | 4:B:2545:TRP:O    | 2.51                     | 0.43              |
| 3:E:929:UNK:HB2   | 3:E:973:UNK:HB2   | 2.00                     | 0.43              |
| 3:E:1538:UNK:HB1  | 3:E:1540:UNK:HG3  | 2.00                     | 0.43              |
| 3:E:1638:UNK:HG2  | 3:E:1707:UNK:HB1  | 2.01                     | 0.43              |
| 4:F:1981:LYS:H    | 4:F:1981:LYS:HG2  | 1.68                     | 0.43              |
| 4:F:2326:VAL:O    | 4:F:2330:VAL:HG23 | 2.19                     | 0.43              |
| 6:H:48:LEU:HB2    | 6:H:317:CYS:HB3   | 2.00                     | 0.43              |
| 1:1:32:UNK:O      | 1:1:33:UNK:C      | 2.66                     | 0.43              |
| 1:1:209:UNK:HB2   | 1:1:330:UNK:HB1   | 2.00                     | 0.43              |
| 1:1:908:UNK:HB1   | 1:1:1006:UNK:HG2  | 2.00                     | 0.43              |
| 1:1:2303:UNK:O    | 1:1:2307:UNK:HB2  | 2.18                     | 0.43              |
| 2:4:97:UNK:HG3    | 2:4:135:UNK:HB2   | 1.99                     | 0.43              |
| 4:B:1500:LYS:HD3  | 4:B:1503:LEU:HD12 | 1.99                     | 0.43              |
| 4:B:1515:MET:H    | 4:B:1515:MET:HG3  | 1.59                     | 0.43              |
| 4:B:1623:LEU:HD13 | 4:B:1640:ARG:HH12 | 1.83                     | 0.43              |
| 4:F:1623:LEU:HD13 | 4:F:1640:ARG:HH12 | 1.83                     | 0.43              |
| 4:F:2260:LEU:HD23 | 4:F:2263:ILE:HA   | 2.01                     | 0.43              |
| 2:2:97:UNK:HG3    | 2:2:135:UNK:HB2   | 1.99                     | 0.43              |
| 2:2:151:UNK:O     | 2:2:152:UNK:C     | 2.65                     | 0.43              |
| 1:3:54:UNK:HA     | 1:3:57:UNK:HB2    | 1.99                     | 0.43              |
| 1:3:706:UNK:HB1   | 1:3:902:UNK:HB1   | 2.00                     | 0.43              |
| 1:3:923:UNK:O     | 1:3:927:UNK:HB1   | 2.18                     | 0.43              |
| 1:3:1310:UNK:CG   | 1:3:1512:UNK:HA   | 2.49                     | 0.43              |
| 3:A:625:UNK:C     | 3:A:627:UNK:H     | 2.31                     | 0.43              |
| 4:B:1575:LEU:O    | 4:B:1578:MET:HG3  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:144:ILE:HG12  | 6:D:185:MET:SD    | 2.59                     | 0.43              |
| 6:D:291:ASP:OD2   | 6:D:295:ARG:NH2   | 2.43                     | 0.43              |
| 3:E:564:UNK:HG3   | 3:E:570:UNK:HG2   | 1.99                     | 0.43              |
| 3:E:932:UNK:O     | 3:E:936:UNK:HG2   | 2.19                     | 0.43              |
| 3:E:992:UNK:HG3   | 3:E:1103:UNK:HG2  | 2.01                     | 0.43              |
| 4:F:1435:TYR:CG   | 4:F:2390:THR:HG21 | 2.53                     | 0.43              |
| 4:F:2297:ASP:O    | 4:F:2301:LYS:HB2  | 2.19                     | 0.43              |
| 4:F:2397:ARG:HA   | 4:F:2400:CYS:SG   | 2.58                     | 0.43              |
| 4:F:2419:GLU:HG2  | 4:F:2501:ILE:CG1  | 2.29                     | 0.43              |
| 5:G:26:UNK:O      | 5:G:39:UNK:N      | 2.50                     | 0.43              |
| 1:3:908:UNK:HB1   | 1:3:1006:UNK:HG2  | 2.01                     | 0.43              |
| 1:3:1913:UNK:HA   | 1:3:2000:UNK:HB2  | 1.99                     | 0.43              |
| 4:B:1575:LEU:HD11 | 4:B:1589:ALA:HB3  | 2.01                     | 0.43              |
| 6:D:267:GLU:O     | 6:D:269:SER:N     | 2.52                     | 0.43              |
| 3:E:773:UNK:O     | 3:E:774:UNK:HB2   | 2.19                     | 0.43              |
| 4:F:1500:LYS:HD3  | 4:F:1503:LEU:HD12 | 1.99                     | 0.43              |
| 4:F:1560:ALA:O    | 4:F:1564:ILE:HG13 | 2.18                     | 0.43              |
| 4:F:2209:LEU:HD23 | 4:F:2406:VAL:HG11 | 2.00                     | 0.43              |
| 4:F:2379:LEU:HD13 | 4:F:2379:LEU:HA   | 1.71                     | 0.43              |
| 1:1:4:UNK:O       | 1:1:7:UNK:HB1     | 2.18                     | 0.43              |
| 1:1:328:UNK:O     | 1:1:331:UNK:HB2   | 2.19                     | 0.43              |
| 1:1:713:UNK:HG1   | 1:1:909:UNK:HB1   | 2.00                     | 0.43              |
| 2:2:168:UNK:O     | 2:2:172:UNK:HG2   | 2.19                     | 0.43              |
| 2:2:607:UNK:HA    | 2:2:610:UNK:HG2   | 2.01                     | 0.43              |
| 1:3:1313:UNK:HG1  | 1:3:1400:UNK:HB1  | 2.00                     | 0.43              |
| 3:A:992:UNK:HG3   | 3:A:1103:UNK:HG2  | 2.01                     | 0.43              |
| 4:B:1437:MET:HE3  | 4:B:1446:GLN:NE2  | 2.34                     | 0.43              |
| 4:B:1444:GLU:O    | 4:B:1445:ILE:HG12 | 2.19                     | 0.43              |
| 4:B:2209:LEU:HD23 | 4:B:2406:VAL:HG11 | 1.99                     | 0.43              |
| 4:B:2214:THR:O    | 4:B:2217:ARG:HB3  | 2.18                     | 0.43              |
| 4:B:2299:LEU:O    | 4:B:2302:LEU:HG   | 2.19                     | 0.43              |
| 4:F:2267:ILE:O    | 4:F:2270:ARG:HB3  | 2.19                     | 0.43              |
| 5:G:4:UNK:HG2     | 5:G:62:UNK:HG3    | 2.00                     | 0.43              |
| 6:H:78:ILE:HB     | 6:H:79:ILE:HG13   | 2.01                     | 0.43              |
| 1:1:923:UNK:O     | 1:1:927:UNK:HB1   | 2.19                     | 0.43              |
| 2:2:109:UNK:O     | 2:2:113:UNK:HB1   | 2.19                     | 0.43              |
| 1:3:1216:UNK:HB1  | 1:3:1305:UNK:HG1  | 2.01                     | 0.43              |
| 4:B:1393:TYR:HD2  | 4:B:1423:LEU:HD13 | 1.83                     | 0.43              |
| 4:B:1951:PRO:HB2  | 4:B:1955:ARG:HH21 | 1.84                     | 0.43              |
| 4:B:2212:ASP:HA   | 4:B:2213:PRO:HD3  | 1.88                     | 0.43              |
| 4:B:2340:HIS:CE1  | 4:B:2342:SER:HB2  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:31:SER:OG    | 6:D:32:GLY:N      | 2.51                     | 0.43              |
| 3:E:578:UNK:O    | 3:E:582:UNK:HG2   | 2.19                     | 0.43              |
| 6:H:142:GLU:OE1  | 6:H:208:THR:HG21  | 2.18                     | 0.43              |
| 1:1:52:UNK:HG1   | 1:1:90:UNK:HB2    | 2.00                     | 0.43              |
| 1:3:319:UNK:O    | 1:3:324:UNK:HB2   | 2.18                     | 0.43              |
| 4:B:1568:ARG:NH2 | 4:B:1600:GLU:OE2  | 2.50                     | 0.43              |
| 4:B:1611:ARG:H   | 4:B:1611:ARG:HG2  | 1.56                     | 0.43              |
| 4:B:2307:SER:OG  | 4:B:2313:TRP:HB2  | 2.19                     | 0.43              |
| 3:E:609:UNK:O    | 3:E:612:UNK:HB1   | 2.19                     | 0.43              |
| 4:F:2254:ARG:HD2 | 4:F:2254:ARG:HA   | 1.57                     | 0.43              |
| 4:F:2277:HIS:HB3 | 6:H:62:TYR:CD1    | 2.53                     | 0.43              |
| 6:H:31:SER:OG    | 6:H:32:GLY:N      | 2.51                     | 0.43              |
| 2:2:163:UNK:O    | 2:2:167:UNK:N     | 2.52                     | 0.42              |
| 2:2:540:UNK:O    | 2:2:543:UNK:HG2   | 2.19                     | 0.42              |
| 1:3:306:UNK:O    | 1:3:310:UNK:HB2   | 2.19                     | 0.42              |
| 4:B:1451:GLU:HG3 | 4:B:1456:TRP:CZ3  | 2.54                     | 0.42              |
| 4:B:1917:PRO:O   | 4:B:1921:GLU:HG3  | 2.19                     | 0.42              |
| 4:B:2315:ASP:O   | 4:B:2318:THR:OG1  | 2.30                     | 0.42              |
| 4:B:2316:ARG:NE  | 4:B:2348:ARG:O    | 2.51                     | 0.42              |
| 4:B:2397:ARG:HB2 | 4:B:2397:ARG:HH11 | 1.84                     | 0.42              |
| 5:C:48:UNK:HG1   | 5:C:55:UNK:HG2    | 2.00                     | 0.42              |
| 6:D:221:ARG:HD3  | 6:D:241:ASP:HA    | 2.01                     | 0.42              |
| 4:F:1393:TYR:HD2 | 4:F:1423:LEU:HD13 | 1.84                     | 0.42              |
| 4:F:2157:ALA:HB3 | 4:F:2173:THR:HG23 | 2.00                     | 0.42              |
| 6:H:132:ASN:ND2  | 6:H:148:GLN:HG2   | 2.34                     | 0.42              |
| 6:H:267:GLU:O    | 6:H:269:SER:N     | 2.52                     | 0.42              |
| 1:1:154:UNK:HG3  | 3:A:643:UNK:CB    | 2.41                     | 0.42              |
| 2:2:79:UNK:HB1   | 2:2:81:UNK:HG3    | 2.01                     | 0.42              |
| 1:3:85:UNK:O     | 1:3:89:UNK:HB1    | 2.19                     | 0.42              |
| 1:3:324:UNK:HG3  | 1:3:427:UNK:HB2   | 2.01                     | 0.42              |
| 2:4:163:UNK:O    | 2:4:167:UNK:N     | 2.52                     | 0.42              |
| 4:B:2267:ILE:O   | 4:B:2270:ARG:HB3  | 2.19                     | 0.42              |
| 4:B:2277:HIS:HB3 | 6:D:62:TYR:CD1    | 2.54                     | 0.42              |
| 6:D:142:GLU:OE1  | 6:D:208:THR:HG21  | 2.19                     | 0.42              |
| 4:F:2214:THR:O   | 4:F:2217:ARG:HB3  | 2.19                     | 0.42              |
| 1:1:510:UNK:HB1  | 1:1:600:UNK:HG1   | 2.01                     | 0.42              |
| 2:4:617:UNK:HA   | 4:F:1393:TYR:CZ   | 2.54                     | 0.42              |
| 3:A:584:UNK:HB1  | 3:A:737:UNK:CG    | 2.45                     | 0.42              |
| 3:A:767:UNK:O    | 3:A:770:UNK:HB2   | 2.20                     | 0.42              |
| 3:A:803:UNK:HB1  | 3:A:1217:UNK:HG2  | 2.00                     | 0.42              |
| 4:B:1513:ALA:CB  | 4:B:1536:ILE:HG12 | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1736:ASP:OD1  | 4:B:1736:ASP:N    | 2.52                     | 0.42              |
| 4:B:2326:VAL:O    | 4:B:2330:VAL:HG23 | 2.19                     | 0.42              |
| 3:E:616:UNK:C     | 3:E:618:UNK:N     | 2.83                     | 0.42              |
| 3:E:635:UNK:HG3   | 3:E:637:UNK:HG2   | 2.01                     | 0.42              |
| 4:F:2185:LEU:HD12 | 4:F:2185:LEU:HA   | 1.80                     | 0.42              |
| 4:F:2288:GLU:O    | 4:F:2292:ASN:ND2  | 2.52                     | 0.42              |
| 6:H:221:ARG:HD3   | 6:H:241:ASP:HA    | 2.02                     | 0.42              |
| 6:H:271:GLY:HA3   | 6:H:290:SER:HB2   | 2.01                     | 0.42              |
| 1:1:32:UNK:O      | 1:1:34:UNK:N      | 2.52                     | 0.42              |
| 1:1:436:UNK:HA    | 1:1:444:UNK:HB2   | 2.00                     | 0.42              |
| 4:B:2218:LYS:HE3  | 4:B:2220:LEU:HD11 | 2.01                     | 0.42              |
| 4:B:2297:ASP:O    | 4:B:2301:LYS:HB2  | 2.19                     | 0.42              |
| 4:B:2397:ARG:HG2  | 4:B:2401:HIS:NE2  | 2.34                     | 0.42              |
| 4:B:2419:GLU:HG2  | 4:B:2501:ILE:CG1  | 2.30                     | 0.42              |
| 6:D:48:LEU:HB2    | 6:D:317:CYS:HB3   | 2.00                     | 0.42              |
| 4:F:1575:LEU:O    | 4:F:1578:MET:HG3  | 2.18                     | 0.42              |
| 4:F:1668:LEU:HD12 | 4:F:1668:LEU:HA   | 1.74                     | 0.42              |
| 6:H:108:THR:OG1   | 6:H:110:ARG:NH1   | 2.52                     | 0.42              |
| 1:1:85:UNK:O      | 1:1:89:UNK:HB1    | 2.19                     | 0.42              |
| 1:1:1913:UNK:HA   | 1:1:2000:UNK:HB2  | 2.00                     | 0.42              |
| 2:2:1:UNK:H       | 2:2:3:UNK:HG2     | 1.85                     | 0.42              |
| 1:3:328:UNK:O     | 1:3:331:UNK:HB2   | 2.19                     | 0.42              |
| 2:4:109:UNK:O     | 2:4:113:UNK:HB1   | 2.19                     | 0.42              |
| 3:A:564:UNK:HG3   | 3:A:570:UNK:HG2   | 2.02                     | 0.42              |
| 4:B:1447:ALA:HB1  | 4:B:1463:TYR:CE2  | 2.55                     | 0.42              |
| 4:B:2157:ALA:HB3  | 4:B:2173:THR:HG23 | 2.00                     | 0.42              |
| 6:D:273:MET:HE2   | 6:D:273:MET:HB2   | 1.94                     | 0.42              |
| 3:E:625:UNK:C     | 3:E:627:UNK:H     | 2.31                     | 0.42              |
| 3:E:721:UNK:HG1   | 3:E:733:UNK:HA    | 2.00                     | 0.42              |
| 4:F:2045:LYS:NZ   | 4:F:2049:GLU:OE2  | 2.43                     | 0.42              |
| 4:F:2074:TYR:HD2  | 4:F:2107:VAL:HG12 | 1.84                     | 0.42              |
| 4:F:2307:SER:OG   | 4:F:2313:TRP:HB2  | 2.20                     | 0.42              |
| 4:F:2340:HIS:CE1  | 4:F:2342:SER:HB2  | 2.54                     | 0.42              |
| 2:2:81:UNK:O      | 2:2:84:UNK:HG2    | 2.20                     | 0.42              |
| 6:D:108:THR:OG1   | 6:D:110:ARG:NH1   | 2.52                     | 0.42              |
| 3:E:581:UNK:O     | 3:E:585:UNK:HB2   | 2.20                     | 0.42              |
| 4:F:1575:LEU:HD11 | 4:F:1589:ALA:HB3  | 2.02                     | 0.42              |
| 4:F:1582:SER:C    | 4:F:1584:SER:H    | 2.27                     | 0.42              |
| 4:F:2132:MET:HE2  | 4:F:2132:MET:HB3  | 1.95                     | 0.42              |
| 4:F:2316:ARG:NE   | 4:F:2348:ARG:O    | 2.53                     | 0.42              |
| 5:G:48:UNK:HG1    | 5:G:55:UNK:HG2    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:306:UNK:O     | 1:1:308:UNK:N     | 2.52                     | 0.42              |
| 1:3:121:UNK:HB1   | 1:3:203:UNK:CB    | 2.50                     | 0.42              |
| 4:B:2260:LEU:HD23 | 4:B:2263:ILE:HA   | 2.00                     | 0.42              |
| 4:B:2288:GLU:O    | 4:B:2292:ASN:ND2  | 2.52                     | 0.42              |
| 4:B:2381:ARG:HA   | 4:B:2384:THR:HB   | 2.02                     | 0.42              |
| 6:D:19:GLY:HA2    | 6:D:316:VAL:HG23  | 2.01                     | 0.42              |
| 6:D:269:SER:C     | 6:D:271:GLY:H     | 2.28                     | 0.42              |
| 4:F:1513:ALA:CB   | 4:F:1536:ILE:HG12 | 2.49                     | 0.42              |
| 4:F:1990:ALA:O    | 4:F:1994:ILE:HG13 | 2.20                     | 0.42              |
| 4:F:2186:LEU:HD12 | 4:F:2186:LEU:HA   | 1.82                     | 0.42              |
| 4:F:2249:LEU:O    | 4:F:2252:ASP:HB2  | 2.20                     | 0.42              |
| 6:H:242:GLN:HG2   | 6:H:271:GLY:O     | 2.20                     | 0.42              |
| 1:1:208:UNK:C     | 1:1:210:UNK:N     | 2.82                     | 0.42              |
| 2:2:549:UNK:HB2   | 4:B:1395:LYS:NZ   | 2.35                     | 0.42              |
| 2:4:168:UNK:O     | 2:4:172:UNK:HG2   | 2.20                     | 0.42              |
| 2:4:540:UNK:O     | 2:4:543:UNK:HG2   | 2.20                     | 0.42              |
| 4:B:1727:GLN:O    | 4:B:1731:ALA:HB3  | 2.20                     | 0.42              |
| 4:B:2341:PRO:HD3  | 4:B:2378:ARG:HH22 | 1.85                     | 0.42              |
| 3:E:117:UNK:HG3   | 3:E:302:UNK:N     | 2.35                     | 0.42              |
| 3:E:985:UNK:O     | 3:E:987:UNK:N     | 2.53                     | 0.42              |
| 4:F:2069:SER:O    | 4:F:2072:GLN:HB2  | 2.20                     | 0.42              |
| 6:H:144:ILE:HG12  | 6:H:185:MET:SD    | 2.59                     | 0.42              |
| 1:3:61:UNK:O      | 1:3:65:UNK:HG2    | 2.20                     | 0.42              |
| 1:3:1913:UNK:O    | 1:3:2116:UNK:HG1  | 2.20                     | 0.42              |
| 3:A:932:UNK:O     | 3:A:936:UNK:HG2   | 2.19                     | 0.42              |
| 4:B:1417:ILE:H    | 4:B:1417:ILE:HG13 | 1.42                     | 0.42              |
| 4:B:1421:ASN:HD21 | 4:B:1452:LYS:HB3  | 1.85                     | 0.42              |
| 4:B:1582:SER:C    | 4:B:1584:SER:H    | 2.28                     | 0.42              |
| 4:B:1607:LEU:O    | 4:B:1608:VAL:HG13 | 2.20                     | 0.42              |
| 6:D:78:ILE:HB     | 6:D:79:ILE:HG13   | 2.01                     | 0.42              |
| 4:F:2397:ARG:NH1  | 4:F:2397:ARG:HB2  | 2.35                     | 0.42              |
| 6:H:40:HIS:CE1    | 6:H:43:SER:HB3    | 2.55                     | 0.42              |
| 1:1:324:UNK:HG3   | 1:1:427:UNK:HB2   | 2.02                     | 0.42              |
| 2:2:515:UNK:O     | 2:2:519:UNK:HG3   | 2.20                     | 0.42              |
| 1:3:117:UNK:C     | 1:3:118:UNK:O     | 2.66                     | 0.42              |
| 1:3:406:UNK:HA    | 1:3:409:UNK:HG2   | 2.02                     | 0.42              |
| 2:4:157:UNK:O     | 2:4:159:UNK:N     | 2.53                     | 0.42              |
| 4:B:2147:ASN:O    | 4:B:2148:GLN:NE2  | 2.31                     | 0.42              |
| 4:B:2250:ILE:O    | 4:B:2254:ARG:HG2  | 2.20                     | 0.42              |
| 5:C:21:UNK:HG3    | 5:C:49:UNK:HG3    | 2.01                     | 0.42              |
| 3:E:405:UNK:HB1   | 3:E:410:UNK:HG1   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:E:1605:UNK:HG3 | 3:E:1611:UNK:HG3  | 2.01                     | 0.42              |
| 4:F:1536:ILE:HA  | 4:F:1537:PRO:HD3  | 1.94                     | 0.42              |
| 4:F:1920:ASN:O   | 4:F:1924:VAL:HG23 | 2.20                     | 0.42              |
| 4:F:1987:ARG:NH1 | 4:F:2426:LEU:HD21 | 2.35                     | 0.42              |
| 4:F:2341:PRO:HD3 | 4:F:2378:ARG:HH22 | 1.84                     | 0.42              |
| 1:1:89:UNK:HG3   | 1:1:90:UNK:HG2    | 2.02                     | 0.41              |
| 2:2:166:UNK:O    | 2:2:169:UNK:HB1   | 2.20                     | 0.41              |
| 2:2:258:UNK:O    | 2:2:261:UNK:HG2   | 2.20                     | 0.41              |
| 2:2:617:UNK:HA   | 4:B:1393:TYR:CZ   | 2.55                     | 0.41              |
| 1:3:4:UNK:O      | 1:3:5:UNK:C       | 2.67                     | 0.41              |
| 1:3:444:UNK:HA   | 1:3:447:UNK:HB1   | 2.02                     | 0.41              |
| 2:4:167:UNK:O    | 2:4:170:UNK:HB2   | 2.20                     | 0.41              |
| 2:4:209:UNK:C    | 2:4:211:UNK:N     | 2.83                     | 0.41              |
| 3:A:405:UNK:HB1  | 3:A:410:UNK:HG1   | 2.01                     | 0.41              |
| 3:A:409:UNK:N    | 3:A:511:UNK:O     | 2.53                     | 0.41              |
| 3:A:635:UNK:HG3  | 3:A:637:UNK:HG2   | 2.02                     | 0.41              |
| 3:A:706:UNK:HB1  | 3:A:707:UNK:H     | 1.66                     | 0.41              |
| 3:A:966:UNK:N    | 3:A:1528:UNK:O    | 2.53                     | 0.41              |
| 3:A:985:UNK:O    | 3:A:987:UNK:N     | 2.53                     | 0.41              |
| 4:B:1701:MET:HE2 | 4:B:1701:MET:HB3  | 1.94                     | 0.41              |
| 4:B:2114:GLN:HG2 | 4:B:2117:GLN:OE1  | 2.20                     | 0.41              |
| 4:B:2397:ARG:NH1 | 4:B:2397:ARG:HB2  | 2.35                     | 0.41              |
| 6:D:313:LYS:HA   | 6:D:313:LYS:HD3   | 1.91                     | 0.41              |
| 4:F:1607:LEU:O   | 4:F:1608:VAL:HG13 | 2.19                     | 0.41              |
| 4:F:1684:GLN:HB3 | 4:F:1687:HIS:HD2  | 1.84                     | 0.41              |
| 4:F:1736:ASP:OD1 | 4:F:1736:ASP:N    | 2.52                     | 0.41              |
| 4:F:2381:ARG:HA  | 4:F:2384:THR:HB   | 2.01                     | 0.41              |
| 4:F:2399:THR:O   | 4:F:2403:VAL:HG23 | 2.20                     | 0.41              |
| 1:1:317:UNK:HG3  | 1:1:318:UNK:O     | 2.19                     | 0.41              |
| 2:2:63:UNK:CG    | 2:2:103:UNK:HG1   | 2.50                     | 0.41              |
| 1:3:89:UNK:HG3   | 1:3:90:UNK:HG2    | 2.01                     | 0.41              |
| 2:4:155:UNK:C    | 2:4:157:UNK:H     | 2.33                     | 0.41              |
| 2:4:166:UNK:O    | 2:4:169:UNK:HB1   | 2.20                     | 0.41              |
| 3:A:117:UNK:HG3  | 3:A:302:UNK:N     | 2.34                     | 0.41              |
| 3:A:549:UNK:HB1  | 3:A:554:UNK:CG    | 2.50                     | 0.41              |
| 3:A:578:UNK:O    | 3:A:582:UNK:HG2   | 2.20                     | 0.41              |
| 3:A:609:UNK:O    | 3:A:612:UNK:HB1   | 2.20                     | 0.41              |
| 4:B:1977:THR:O   | 4:B:1981:LYS:HE2  | 2.21                     | 0.41              |
| 4:B:2154:GLN:N   | 4:B:2175:MET:O    | 2.50                     | 0.41              |
| 3:E:1343:UNK:HA  | 3:E:1368:UNK:O    | 2.20                     | 0.41              |
| 4:F:1611:ARG:H   | 4:F:1611:ARG:HG2  | 1.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:F:2411:LYS:HB2 | 4:F:2411:LYS:HE3  | 1.69                     | 0.41              |
| 2:2:155:UNK:C    | 2:2:157:UNK:H     | 2.34                     | 0.41              |
| 2:2:211:UNK:HA   | 2:2:214:UNK:HG3   | 2.02                     | 0.41              |
| 2:4:108:UNK:O    | 2:4:112:UNK:HG2   | 2.21                     | 0.41              |
| 2:4:211:UNK:O    | 2:4:214:UNK:N     | 2.53                     | 0.41              |
| 3:A:773:UNK:O    | 3:A:774:UNK:HB2   | 2.20                     | 0.41              |
| 3:A:1531:UNK:HG3 | 3:A:1532:UNK:HG2  | 2.01                     | 0.41              |
| 4:B:2399:THR:O   | 4:B:2403:VAL:HG23 | 2.19                     | 0.41              |
| 6:D:242:GLN:HG2  | 6:D:271:GLY:O     | 2.20                     | 0.41              |
| 3:E:409:UNK:N    | 3:E:511:UNK:O     | 2.52                     | 0.41              |
| 3:E:1531:UNK:HG3 | 3:E:1532:UNK:HG2  | 2.02                     | 0.41              |
| 4:F:1451:GLU:HG3 | 4:F:1456:TRP:CZ3  | 2.55                     | 0.41              |
| 4:F:1917:PRO:O   | 4:F:1921:GLU:HG3  | 2.19                     | 0.41              |
| 4:F:2503:ARG:O   | 4:F:2506:ASP:HB2  | 2.21                     | 0.41              |
| 6:H:101:TYR:CD1  | 6:H:111:ILE:HG12  | 2.56                     | 0.41              |
| 2:2:167:UNK:O    | 2:2:170:UNK:HB2   | 2.20                     | 0.41              |
| 2:4:60:UNK:O     | 2:4:64:UNK:HG3    | 2.21                     | 0.41              |
| 2:4:81:UNK:O     | 2:4:84:UNK:HG2    | 2.19                     | 0.41              |
| 3:A:616:UNK:C    | 3:A:618:UNK:N     | 2.82                     | 0.41              |
| 3:A:721:UNK:HG1  | 3:A:733:UNK:HA    | 2.01                     | 0.41              |
| 3:A:1387:UNK:HG1 | 3:A:1502:UNK:HB1  | 2.02                     | 0.41              |
| 4:B:1684:GLN:HB3 | 4:B:1687:HIS:HD2  | 1.84                     | 0.41              |
| 4:F:1417:ILE:H   | 4:F:1417:ILE:HG13 | 1.41                     | 0.41              |
| 4:F:2250:ILE:O   | 4:F:2254:ARG:HG2  | 2.20                     | 0.41              |
| 4:F:2340:HIS:O   | 4:F:2343:ASN:N    | 2.46                     | 0.41              |
| 1:1:42:UNK:HB2   | 4:F:1611:ARG:HH12 | 1.84                     | 0.41              |
| 1:1:117:UNK:C    | 1:1:118:UNK:O     | 2.66                     | 0.41              |
| 1:1:444:UNK:HA   | 1:1:447:UNK:HB1   | 2.02                     | 0.41              |
| 1:1:1909:UNK:O   | 1:1:1913:UNK:HB2  | 2.20                     | 0.41              |
| 2:2:60:UNK:O     | 2:2:64:UNK:HG3    | 2.21                     | 0.41              |
| 2:2:184:UNK:O    | 2:2:188:UNK:N     | 2.53                     | 0.41              |
| 2:2:192:UNK:O    | 2:2:196:UNK:HG3   | 2.20                     | 0.41              |
| 2:2:302:UNK:O    | 2:2:305:UNK:HB2   | 2.21                     | 0.41              |
| 1:3:317:UNK:HG3  | 1:3:318:UNK:O     | 2.20                     | 0.41              |
| 1:3:425:UNK:HA   | 1:3:428:UNK:HB2   | 2.03                     | 0.41              |
| 1:3:2213:UNK:HG1 | 1:3:2309:UNK:HG1  | 2.02                     | 0.41              |
| 2:4:63:UNK:CG    | 2:4:103:UNK:HG1   | 2.50                     | 0.41              |
| 2:4:268:UNK:C    | 2:4:270:UNK:N     | 2.83                     | 0.41              |
| 2:4:549:UNK:HB2  | 4:F:1395:LYS:NZ   | 2.35                     | 0.41              |
| 3:A:1638:UNK:HB2 | 3:A:1643:UNK:O    | 2.20                     | 0.41              |
| 4:B:1670:HIS:HD2 | 4:B:1703:ASN:HD21 | 1.69                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:1920:ASN:O   | 4:B:1924:VAL:HG23 | 2.20                     | 0.41              |
| 3:E:767:UNK:O    | 3:E:770:UNK:HB2   | 2.19                     | 0.41              |
| 3:E:966:UNK:N    | 3:E:1528:UNK:O    | 2.53                     | 0.41              |
| 4:F:2060:ARG:NH2 | 4:F:2061:GLY:O    | 2.30                     | 0.41              |
| 4:F:2114:GLN:HG2 | 4:F:2117:GLN:OE1  | 2.20                     | 0.41              |
| 1:1:13:UNK:HB1   | 1:1:21:UNK:HG3    | 2.02                     | 0.41              |
| 2:2:157:UNK:O    | 2:2:159:UNK:N     | 2.54                     | 0.41              |
| 1:3:13:UNK:HB1   | 1:3:21:UNK:HG3    | 2.03                     | 0.41              |
| 1:3:1909:UNK:O   | 1:3:1913:UNK:HB2  | 2.21                     | 0.41              |
| 2:4:192:UNK:O    | 2:4:196:UNK:HG3   | 2.20                     | 0.41              |
| 2:4:206:UNK:O    | 2:4:209:UNK:HB1   | 2.21                     | 0.41              |
| 2:4:212:UNK:HG1  | 2:4:225:UNK:HG1   | 2.01                     | 0.41              |
| 3:A:1523:UNK:HG3 | 3:A:1530:UNK:HG2  | 2.03                     | 0.41              |
| 4:B:1434:GLU:O   | 4:B:1438:LYS:HD2  | 2.21                     | 0.41              |
| 4:B:1541:HIS:CG  | 4:B:1542:ASP:N    | 2.89                     | 0.41              |
| 4:B:2541:CYS:HB3 | 4:B:2547:PRO:HG3  | 2.02                     | 0.41              |
| 3:E:245:UNK:HA   | 3:E:248:UNK:HB1   | 2.02                     | 0.41              |
| 4:F:2370:LYS:HA  | 4:F:2370:LYS:HD2  | 1.86                     | 0.41              |
| 5:G:21:UNK:HG3   | 5:G:49:UNK:HG3    | 2.02                     | 0.41              |
| 1:1:28:UNK:HA    | 1:1:31:UNK:HB2    | 2.01                     | 0.41              |
| 1:1:106:UNK:O    | 1:1:109:UNK:HB1   | 2.20                     | 0.41              |
| 1:1:121:UNK:HB1  | 1:1:203:UNK:CB    | 2.50                     | 0.41              |
| 2:2:211:UNK:O    | 2:2:214:UNK:N     | 2.54                     | 0.41              |
| 1:3:42:UNK:HB2   | 4:B:1611:ARG:HH12 | 1.86                     | 0.41              |
| 1:3:106:UNK:O    | 1:3:109:UNK:HB1   | 2.20                     | 0.41              |
| 1:3:510:UNK:HB1  | 1:3:600:UNK:HG1   | 2.02                     | 0.41              |
| 2:4:117:UNK:C    | 2:4:119:UNK:N     | 2.84                     | 0.41              |
| 2:4:515:UNK:O    | 2:4:519:UNK:HG3   | 2.19                     | 0.41              |
| 2:4:611:UNK:C    | 2:4:613:UNK:N     | 2.83                     | 0.41              |
| 3:A:1514:UNK:HB1 | 3:A:1542:UNK:HB1  | 2.02                     | 0.41              |
| 4:B:1571:LEU:O   | 4:B:1574:GLU:HB3  | 2.20                     | 0.41              |
| 4:B:1701:MET:HE1 | 4:B:1717:MET:N    | 2.36                     | 0.41              |
| 4:B:1990:ALA:O   | 4:B:1994:ILE:HG13 | 2.20                     | 0.41              |
| 4:B:2074:TYR:HD2 | 4:B:2107:VAL:HG12 | 1.84                     | 0.41              |
| 4:B:2249:LEU:O   | 4:B:2252:ASP:HB2  | 2.20                     | 0.41              |
| 4:F:1401:GLU:O   | 4:F:1404:PHE:HB3  | 2.21                     | 0.41              |
| 4:F:2218:LYS:HE3 | 4:F:2220:LEU:HD11 | 2.01                     | 0.41              |
| 1:1:435:UNK:CG   | 1:1:447:UNK:HG1   | 2.51                     | 0.41              |
| 2:2:209:UNK:C    | 2:2:211:UNK:N     | 2.83                     | 0.41              |
| 4:B:2069:SER:O   | 4:B:2072:GLN:HB2  | 2.20                     | 0.41              |
| 4:B:2166:LYS:HD2 | 4:B:2166:LYS:HA   | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:2256:LYS:NZ   | 4:B:2257:LYS:HE3  | 2.34                     | 0.41              |
| 4:B:2423:TYR:CE2  | 4:B:2501:ILE:HD13 | 2.56                     | 0.41              |
| 4:F:2374:LYS:HA   | 4:F:2374:LYS:HD3  | 1.89                     | 0.41              |
| 6:H:78:ILE:H      | 6:H:78:ILE:HG13   | 1.60                     | 0.41              |
| 6:H:113:ASP:HB3   | 6:H:116:SER:OG    | 2.21                     | 0.41              |
| 1:1:416:UNK:C     | 1:1:418:UNK:N     | 2.84                     | 0.41              |
| 1:1:507:UNK:O     | 1:1:511:UNK:HG2   | 2.21                     | 0.41              |
| 2:2:63:UNK:HG1    | 2:2:103:UNK:HG1   | 2.02                     | 0.41              |
| 2:2:106:UNK:O     | 2:2:110:UNK:HG2   | 2.21                     | 0.41              |
| 2:2:116:UNK:HG3   | 2:2:119:UNK:HB1   | 2.02                     | 0.41              |
| 2:2:507:UNK:O     | 2:2:511:UNK:HG2   | 2.21                     | 0.41              |
| 1:3:1:UNK:HA      | 4:B:1622:ARG:NE   | 2.36                     | 0.41              |
| 1:3:33:UNK:HB2    | 1:3:34:UNK:H      | 1.55                     | 0.41              |
| 1:3:48:UNK:HA     | 1:3:51:UNK:CB     | 2.51                     | 0.41              |
| 2:4:184:UNK:O     | 2:4:188:UNK:N     | 2.54                     | 0.41              |
| 2:4:197:UNK:O     | 2:4:201:UNK:HG3   | 2.21                     | 0.41              |
| 2:4:203:UNK:O     | 2:4:206:UNK:HB1   | 2.20                     | 0.41              |
| 2:4:208:UNK:O     | 2:4:212:UNK:HG3   | 2.21                     | 0.41              |
| 3:A:517:UNK:C     | 3:A:519:UNK:N     | 2.84                     | 0.41              |
| 3:A:577:UNK:HG2   | 3:A:741:UNK:HB1   | 2.03                     | 0.41              |
| 4:B:1890:ARG:O    | 4:B:1893:SER:OG   | 2.31                     | 0.41              |
| 4:B:1987:ARG:NH1  | 4:B:2426:LEU:HD21 | 2.35                     | 0.41              |
| 4:B:2090:LYS:HE2  | 4:B:2090:LYS:HB2  | 1.91                     | 0.41              |
| 4:B:2370:LYS:HA   | 4:B:2370:LYS:HD2  | 1.85                     | 0.41              |
| 4:B:2503:ARG:O    | 4:B:2506:ASP:HB2  | 2.20                     | 0.41              |
| 6:D:101:TYR:CD1   | 6:D:111:ILE:HG12  | 2.55                     | 0.41              |
| 3:E:758:UNK:O     | 3:E:762:UNK:HG2   | 2.21                     | 0.41              |
| 3:E:906:UNK:HA    | 3:E:909:UNK:HB2   | 2.03                     | 0.41              |
| 3:E:1387:UNK:HG1  | 3:E:1502:UNK:HB1  | 2.02                     | 0.41              |
| 4:F:1434:GLU:O    | 4:F:1438:LYS:HD2  | 2.20                     | 0.41              |
| 4:F:1608:VAL:HA   | 4:F:1609:PRO:HD3  | 1.77                     | 0.41              |
| 4:F:1623:LEU:HD12 | 4:F:1623:LEU:HA   | 1.95                     | 0.41              |
| 4:F:1673:LEU:HD13 | 4:F:1700:TYR:HD1  | 1.86                     | 0.41              |
| 4:F:1770:PRO:HA   | 4:F:1773:LEU:HB2  | 2.02                     | 0.41              |
| 1:1:61:UNK:O      | 1:1:65:UNK:HG2    | 2.20                     | 0.41              |
| 1:1:1913:UNK:O    | 1:1:2116:UNK:HG1  | 2.20                     | 0.41              |
| 2:2:203:UNK:O     | 2:2:206:UNK:HB1   | 2.20                     | 0.41              |
| 2:2:212:UNK:HG1   | 2:2:225:UNK:HG1   | 2.02                     | 0.41              |
| 1:3:209:UNK:HB2   | 1:3:330:UNK:HB1   | 2.01                     | 0.41              |
| 1:3:507:UNK:O     | 1:3:511:UNK:HG2   | 2.21                     | 0.41              |
| 2:4:79:UNK:HB1    | 2:4:81:UNK:HG3    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4:106:UNK:O     | 2:4:110:UNK:HG2   | 2.21                     | 0.41              |
| 3:A:846:UNK:O     | 3:A:849:UNK:HB2   | 2.21                     | 0.41              |
| 3:A:906:UNK:HA    | 3:A:909:UNK:HB2   | 2.03                     | 0.41              |
| 3:A:913:UNK:O     | 3:A:917:UNK:HG2   | 2.22                     | 0.41              |
| 3:A:1343:UNK:HA   | 3:A:1368:UNK:O    | 2.20                     | 0.41              |
| 4:B:2253:TYR:CE1  | 4:B:2257:LYS:HG3  | 2.56                     | 0.41              |
| 3:E:963:UNK:HG3   | 3:E:1112:UNK:HG1  | 2.03                     | 0.41              |
| 3:E:1544:UNK:HG3  | 3:E:1558:UNK:HG3  | 2.03                     | 0.41              |
| 4:F:1397:LEU:HD12 | 4:F:1397:LEU:HA   | 1.81                     | 0.41              |
| 4:F:2343:ASN:HD22 | 4:F:2343:ASN:HA   | 1.70                     | 0.41              |
| 2:2:21:UNK:O      | 2:2:25:UNK:HB1    | 2.21                     | 0.40              |
| 2:2:268:UNK:C     | 2:2:270:UNK:N     | 2.83                     | 0.40              |
| 2:2:552:UNK:HG1   | 4:B:2304:TRP:CZ2  | 2.44                     | 0.40              |
| 1:3:208:UNK:C     | 1:3:210:UNK:N     | 2.83                     | 0.40              |
| 2:4:258:UNK:O     | 2:4:261:UNK:HG2   | 2.20                     | 0.40              |
| 3:A:1605:UNK:HG3  | 3:A:1611:UNK:HG3  | 2.02                     | 0.40              |
| 4:F:1977:THR:O    | 4:F:1981:LYS:HE2  | 2.20                     | 0.40              |
| 4:F:2256:LYS:NZ   | 4:F:2257:LYS:HE3  | 2.34                     | 0.40              |
| 4:F:2424:ASP:CG   | 4:F:2425:PRO:HD2  | 2.46                     | 0.40              |
| 5:G:81:UNK:HG1    | 5:G:97:UNK:HB2    | 2.03                     | 0.40              |
| 6:H:269:SER:C     | 6:H:271:GLY:H     | 2.28                     | 0.40              |
| 2:2:197:UNK:O     | 2:2:201:UNK:HG3   | 2.21                     | 0.40              |
| 1:3:28:UNK:HA     | 1:3:31:UNK:HB2    | 2.02                     | 0.40              |
| 2:4:1:UNK:H       | 2:4:3:UNK:HG2     | 1.86                     | 0.40              |
| 2:4:607:UNK:HA    | 2:4:610:UNK:HG2   | 2.03                     | 0.40              |
| 3:A:315:UNK:O     | 3:A:317:UNK:HG2   | 2.21                     | 0.40              |
| 3:A:557:UNK:HG2   | 3:A:652:UNK:HG1   | 2.03                     | 0.40              |
| 4:B:1433:LEU:HD22 | 4:B:1453:LEU:HG   | 2.03                     | 0.40              |
| 4:B:2431:LEU:HB2  | 4:B:2493:LEU:HD22 | 2.03                     | 0.40              |
| 5:C:60:UNK:O      | 5:C:64:UNK:HB2    | 2.22                     | 0.40              |
| 6:D:50:VAL:HG23   | 6:D:319:ALA:HB1   | 2.03                     | 0.40              |
| 3:E:913:UNK:O     | 3:E:917:UNK:HG2   | 2.22                     | 0.40              |
| 4:F:1447:ALA:HB1  | 4:F:1463:TYR:CE2  | 2.56                     | 0.40              |
| 4:F:1670:HIS:HD2  | 4:F:1703:ASN:HD21 | 1.70                     | 0.40              |
| 4:F:1701:MET:HE2  | 4:F:1701:MET:HB3  | 1.94                     | 0.40              |
| 4:F:2170:ARG:HB2  | 4:F:2186:LEU:HB3  | 2.03                     | 0.40              |
| 5:G:60:UNK:O      | 5:G:64:UNK:HB2    | 2.22                     | 0.40              |
| 1:1:2213:UNK:HG1  | 1:1:2309:UNK:HG1  | 2.02                     | 0.40              |
| 2:2:78:UNK:HB1    | 3:A:634:UNK:HA    | 2.02                     | 0.40              |
| 2:2:108:UNK:O     | 2:2:112:UNK:HG2   | 2.21                     | 0.40              |
| 2:2:208:UNK:O     | 2:2:212:UNK:HG3   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4:552:UNK:CG    | 4:F:2304:TRP:HZ2  | 2.26                     | 0.40              |
| 3:A:114:UNK:HG2   | 3:A:300:UNK:C     | 2.52                     | 0.40              |
| 4:B:1756:GLU:O    | 4:B:1759:LEU:HB2  | 2.22                     | 0.40              |
| 6:D:113:ASP:HB3   | 6:D:116:SER:OG    | 2.21                     | 0.40              |
| 6:D:248:ARG:H     | 6:D:248:ARG:HG2   | 1.73                     | 0.40              |
| 3:E:318:UNK:HG1   | 3:E:333:UNK:HB1   | 2.03                     | 0.40              |
| 3:E:1638:UNK:HB2  | 3:E:1643:UNK:O    | 2.20                     | 0.40              |
| 3:E:1641:UNK:HG3  | 3:E:1643:UNK:HB2  | 2.03                     | 0.40              |
| 4:F:1756:GLU:O    | 4:F:1759:LEU:HB2  | 2.22                     | 0.40              |
| 4:F:1881:THR:O    | 4:F:1884:ALA:HB3  | 2.22                     | 0.40              |
| 4:F:2431:LEU:HB2  | 4:F:2493:LEU:HD22 | 2.03                     | 0.40              |
| 4:F:2515:HIS:HD1  | 4:F:2516:ASP:N    | 2.20                     | 0.40              |
| 1:1:425:UNK:HA    | 1:1:428:UNK:HB2   | 2.03                     | 0.40              |
| 3:A:318:UNK:HG1   | 3:A:333:UNK:HB1   | 2.03                     | 0.40              |
| 3:A:712:UNK:HG2   | 3:A:748:UNK:HG1   | 2.03                     | 0.40              |
| 3:A:963:UNK:HG3   | 3:A:1112:UNK:HG1  | 2.04                     | 0.40              |
| 3:A:1544:UNK:HG3  | 3:A:1558:UNK:HG3  | 2.03                     | 0.40              |
| 3:A:1641:UNK:HG3  | 3:A:1643:UNK:HB2  | 2.03                     | 0.40              |
| 4:B:2185:LEU:HA   | 4:B:2185:LEU:HD12 | 1.81                     | 0.40              |
| 5:C:54:UNK:O      | 7:C:999:RAP:O10   | 2.40                     | 0.40              |
| 6:D:125:PHE:HB2   | 6:D:155:TRP:CZ2   | 2.56                     | 0.40              |
| 6:D:195:TYR:CE2   | 6:D:215:LYS:HG3   | 2.56                     | 0.40              |
| 3:E:549:UNK:HB1   | 3:E:554:UNK:CG    | 2.51                     | 0.40              |
| 4:F:1727:GLN:O    | 4:F:1731:ALA:HB3  | 2.20                     | 0.40              |
| 4:F:1743:LEU:HD12 | 4:F:1743:LEU:HA   | 1.96                     | 0.40              |
| 4:F:2154:GLN:N    | 4:F:2175:MET:O    | 2.51                     | 0.40              |
| 1:1:1:UNK:HA      | 4:F:1622:ARG:NE   | 2.36                     | 0.40              |
| 1:1:80:UNK:C      | 1:1:82:UNK:N      | 2.85                     | 0.40              |
| 2:2:100:UNK:C     | 2:2:102:UNK:N     | 2.85                     | 0.40              |
| 2:4:302:UNK:O     | 2:4:305:UNK:HB2   | 2.21                     | 0.40              |
| 3:A:758:UNK:O     | 3:A:762:UNK:HG2   | 2.21                     | 0.40              |
| 4:B:2011:MET:HE1  | 4:B:2133:CYS:SG   | 2.62                     | 0.40              |
| 4:B:2039:PHE:CZ   | 7:C:999:RAP:H502  | 2.57                     | 0.40              |
| 4:B:2051:LEU:HD12 | 4:B:2051:LEU:HA   | 1.80                     | 0.40              |
| 4:B:2303:LEU:HA   | 4:B:2303:LEU:HD23 | 1.80                     | 0.40              |
| 3:E:1524:UNK:O    | 3:E:1528:UNK:N    | 2.55                     | 0.40              |
| 4:F:2242:HIS:HA   | 4:F:2348:ARG:NH1  | 2.37                     | 0.40              |
| 4:F:2247:HIS:HA   | 4:F:2549:TRP:HZ3  | 1.87                     | 0.40              |
| 6:H:125:PHE:HB2   | 6:H:155:TRP:CZ2   | 2.56                     | 0.40              |
| 6:H:168:GLU:HA    | 6:H:169:PRO:HD3   | 1.93                     | 0.40              |
| 6:H:273:MET:HE2   | 6:H:273:MET:HB2   | 1.94                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 4   | B     | 1045/1168 (90%) | 996 (95%)  | 47 (4%)  | 2 (0%)   | 43          | 77 |
| 4   | F     | 1045/1168 (90%) | 997 (95%)  | 46 (4%)  | 2 (0%)   | 43          | 77 |
| 6   | D     | 315/326 (97%)   | 293 (93%)  | 21 (7%)  | 1 (0%)   | 36          | 72 |
| 6   | H     | 315/326 (97%)   | 293 (93%)  | 21 (7%)  | 1 (0%)   | 36          | 72 |
| All | All   | 2720/2988 (91%) | 2579 (95%) | 135 (5%) | 6 (0%)   | 44          | 77 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 268  | SER  |
| 6   | H     | 268  | SER  |
| 4   | B     | 1578 | MET  |
| 4   | F     | 1578 | MET  |
| 4   | B     | 1679 | VAL  |
| 4   | F     | 1679 | VAL  |

### 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 |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 4   | B     | 927/1019 (91%) | 820 (88%) | 107 (12%) | 5           | 18 |
| 4   | F     | 927/1019 (91%) | 821 (89%) | 106 (11%) | 5           | 18 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 6   | D     | 269/276 (98%)   | 246 (91%)  | 23 (9%)   | 10          | 29 |
| 6   | H     | 269/276 (98%)   | 246 (91%)  | 23 (9%)   | 10          | 29 |
| All | All   | 2392/2590 (92%) | 2133 (89%) | 259 (11%) | 8           | 21 |

All (259) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1393 | TYR  |
| 4   | B     | 1416 | LEU  |
| 4   | B     | 1417 | ILE  |
| 4   | B     | 1422 | LYS  |
| 4   | B     | 1424 | GLN  |
| 4   | B     | 1425 | GLN  |
| 4   | B     | 1427 | GLU  |
| 4   | B     | 1443 | LEU  |
| 4   | B     | 1445 | ILE  |
| 4   | B     | 1449 | TRP  |
| 4   | B     | 1453 | LEU  |
| 4   | B     | 1458 | ASP  |
| 4   | B     | 1463 | TYR  |
| 4   | B     | 1489 | GLU  |
| 4   | B     | 1535 | MET  |
| 4   | B     | 1536 | ILE  |
| 4   | B     | 1541 | HIS  |
| 4   | B     | 1547 | ARG  |
| 4   | B     | 1559 | LEU  |
| 4   | B     | 1563 | CYS  |
| 4   | B     | 1565 | ASP  |
| 4   | B     | 1571 | LEU  |
| 4   | B     | 1583 | TYR  |
| 4   | B     | 1585 | ARG  |
| 4   | B     | 1587 | TYR  |
| 4   | B     | 1599 | LEU  |
| 4   | B     | 1608 | VAL  |
| 4   | B     | 1611 | ARG  |
| 4   | B     | 1614 | ILE  |
| 4   | B     | 1622 | ARG  |
| 4   | B     | 1627 | GLN  |
| 4   | B     | 1629 | ILE  |
| 4   | B     | 1630 | VAL  |
| 4   | B     | 1633 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1642 | LEU  |
| 4   | B     | 1643 | VAL  |
| 4   | B     | 1659 | LEU  |
| 4   | B     | 1668 | LEU  |
| 4   | B     | 1677 | LEU  |
| 4   | B     | 1679 | VAL  |
| 4   | B     | 1695 | GLN  |
| 4   | B     | 1702 | LYS  |
| 4   | B     | 1710 | LYS  |
| 4   | B     | 1732 | ILE  |
| 4   | B     | 1736 | ASP  |
| 4   | B     | 1758 | GLN  |
| 4   | B     | 1780 | THR  |
| 4   | B     | 1899 | ASN  |
| 4   | B     | 1902 | ASP  |
| 4   | B     | 1907 | LEU  |
| 4   | B     | 1918 | ASP  |
| 4   | B     | 1925 | GLU  |
| 4   | B     | 1938 | VAL  |
| 4   | B     | 1956 | LEU  |
| 4   | B     | 1973 | ILE  |
| 4   | B     | 1984 | THR  |
| 4   | B     | 1985 | THR  |
| 4   | B     | 2005 | LEU  |
| 4   | B     | 2010 | MET  |
| 4   | B     | 2011 | MET  |
| 4   | B     | 2021 | ILE  |
| 4   | B     | 2033 | GLU  |
| 4   | B     | 2044 | VAL  |
| 4   | B     | 2090 | LYS  |
| 4   | B     | 2093 | ASN  |
| 4   | B     | 2099 | GLN  |
| 4   | B     | 2115 | LEU  |
| 4   | B     | 2122 | GLU  |
| 4   | B     | 2123 | LEU  |
| 4   | B     | 2133 | CYS  |
| 4   | B     | 2138 | LEU  |
| 4   | B     | 2145 | ASP  |
| 4   | B     | 2152 | ARG  |
| 4   | B     | 2173 | THR  |
| 4   | B     | 2178 | ASN  |
| 4   | B     | 2185 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 2189 | HIS  |
| 4   | B     | 2201 | LEU  |
| 4   | B     | 2223 | GLN  |
| 4   | B     | 2228 | ILE  |
| 4   | B     | 2240 | VAL  |
| 4   | B     | 2245 | THR  |
| 4   | B     | 2250 | ILE  |
| 4   | B     | 2254 | ARG  |
| 4   | B     | 2255 | GLU  |
| 4   | B     | 2266 | ARG  |
| 4   | B     | 2306 | LYS  |
| 4   | B     | 2318 | THR  |
| 4   | B     | 2321 | THR  |
| 4   | B     | 2323 | SER  |
| 4   | B     | 2333 | ILE  |
| 4   | B     | 2339 | ARG  |
| 4   | B     | 2343 | ASN  |
| 4   | B     | 2363 | GLU  |
| 4   | B     | 2367 | THR  |
| 4   | B     | 2368 | ARG  |
| 4   | B     | 2379 | LEU  |
| 4   | B     | 2393 | ASP  |
| 4   | B     | 2405 | GLU  |
| 4   | B     | 2412 | ASP  |
| 4   | B     | 2415 | MET  |
| 4   | B     | 2424 | ASP  |
| 4   | B     | 2501 | ILE  |
| 4   | B     | 2503 | ARG  |
| 4   | B     | 2530 | LYS  |
| 4   | B     | 2543 | ILE  |
| 4   | B     | 2548 | PHE  |
| 6   | D     | 44   | GLN  |
| 6   | D     | 53   | ASP  |
| 6   | D     | 78   | ILE  |
| 6   | D     | 84   | VAL  |
| 6   | D     | 106  | ASP  |
| 6   | D     | 159  | THR  |
| 6   | D     | 162  | ASN  |
| 6   | D     | 164  | GLN  |
| 6   | D     | 171  | VAL  |
| 6   | D     | 173  | ILE  |
| 6   | D     | 179  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 188  | VAL  |
| 6   | D     | 197  | TRP  |
| 6   | D     | 199  | LEU  |
| 6   | D     | 243  | THR  |
| 6   | D     | 251  | ASN  |
| 6   | D     | 260  | ILE  |
| 6   | D     | 273  | MET  |
| 6   | D     | 287  | THR  |
| 6   | D     | 292  | ASN  |
| 6   | D     | 308  | TYR  |
| 6   | D     | 312  | GLN  |
| 6   | D     | 316  | VAL  |
| 4   | F     | 1393 | TYR  |
| 4   | F     | 1416 | LEU  |
| 4   | F     | 1417 | ILE  |
| 4   | F     | 1422 | LYS  |
| 4   | F     | 1424 | GLN  |
| 4   | F     | 1425 | GLN  |
| 4   | F     | 1427 | GLU  |
| 4   | F     | 1443 | LEU  |
| 4   | F     | 1445 | ILE  |
| 4   | F     | 1449 | TRP  |
| 4   | F     | 1453 | LEU  |
| 4   | F     | 1458 | ASP  |
| 4   | F     | 1463 | TYR  |
| 4   | F     | 1489 | GLU  |
| 4   | F     | 1535 | MET  |
| 4   | F     | 1536 | ILE  |
| 4   | F     | 1541 | HIS  |
| 4   | F     | 1547 | ARG  |
| 4   | F     | 1559 | LEU  |
| 4   | F     | 1563 | CYS  |
| 4   | F     | 1565 | ASP  |
| 4   | F     | 1571 | LEU  |
| 4   | F     | 1585 | ARG  |
| 4   | F     | 1587 | TYR  |
| 4   | F     | 1599 | LEU  |
| 4   | F     | 1608 | VAL  |
| 4   | F     | 1611 | ARG  |
| 4   | F     | 1614 | ILE  |
| 4   | F     | 1622 | ARG  |
| 4   | F     | 1629 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | F     | 1630 | VAL  |
| 4   | F     | 1633 | TRP  |
| 4   | F     | 1636 | ILE  |
| 4   | F     | 1642 | LEU  |
| 4   | F     | 1643 | VAL  |
| 4   | F     | 1659 | LEU  |
| 4   | F     | 1668 | LEU  |
| 4   | F     | 1677 | LEU  |
| 4   | F     | 1679 | VAL  |
| 4   | F     | 1695 | GLN  |
| 4   | F     | 1702 | LYS  |
| 4   | F     | 1710 | LYS  |
| 4   | F     | 1732 | ILE  |
| 4   | F     | 1736 | ASP  |
| 4   | F     | 1758 | GLN  |
| 4   | F     | 1780 | THR  |
| 4   | F     | 1899 | ASN  |
| 4   | F     | 1902 | ASP  |
| 4   | F     | 1907 | LEU  |
| 4   | F     | 1918 | ASP  |
| 4   | F     | 1925 | GLU  |
| 4   | F     | 1938 | VAL  |
| 4   | F     | 1956 | LEU  |
| 4   | F     | 1973 | ILE  |
| 4   | F     | 1984 | THR  |
| 4   | F     | 1985 | THR  |
| 4   | F     | 2005 | LEU  |
| 4   | F     | 2010 | MET  |
| 4   | F     | 2011 | MET  |
| 4   | F     | 2021 | ILE  |
| 4   | F     | 2033 | GLU  |
| 4   | F     | 2044 | VAL  |
| 4   | F     | 2090 | LYS  |
| 4   | F     | 2093 | ASN  |
| 4   | F     | 2099 | GLN  |
| 4   | F     | 2115 | LEU  |
| 4   | F     | 2122 | GLU  |
| 4   | F     | 2123 | LEU  |
| 4   | F     | 2133 | CYS  |
| 4   | F     | 2138 | LEU  |
| 4   | F     | 2145 | ASP  |
| 4   | F     | 2152 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | F     | 2173 | THR  |
| 4   | F     | 2178 | ASN  |
| 4   | F     | 2185 | LEU  |
| 4   | F     | 2189 | HIS  |
| 4   | F     | 2201 | LEU  |
| 4   | F     | 2223 | GLN  |
| 4   | F     | 2228 | ILE  |
| 4   | F     | 2240 | VAL  |
| 4   | F     | 2245 | THR  |
| 4   | F     | 2250 | ILE  |
| 4   | F     | 2254 | ARG  |
| 4   | F     | 2255 | GLU  |
| 4   | F     | 2266 | ARG  |
| 4   | F     | 2306 | LYS  |
| 4   | F     | 2318 | THR  |
| 4   | F     | 2321 | THR  |
| 4   | F     | 2323 | SER  |
| 4   | F     | 2333 | ILE  |
| 4   | F     | 2339 | ARG  |
| 4   | F     | 2343 | ASN  |
| 4   | F     | 2363 | GLU  |
| 4   | F     | 2367 | THR  |
| 4   | F     | 2368 | ARG  |
| 4   | F     | 2379 | LEU  |
| 4   | F     | 2393 | ASP  |
| 4   | F     | 2405 | GLU  |
| 4   | F     | 2412 | ASP  |
| 4   | F     | 2415 | MET  |
| 4   | F     | 2424 | ASP  |
| 4   | F     | 2501 | ILE  |
| 4   | F     | 2503 | ARG  |
| 4   | F     | 2530 | LYS  |
| 4   | F     | 2543 | ILE  |
| 4   | F     | 2548 | PHE  |
| 6   | H     | 44   | GLN  |
| 6   | H     | 53   | ASP  |
| 6   | H     | 78   | ILE  |
| 6   | H     | 84   | VAL  |
| 6   | H     | 106  | ASP  |
| 6   | H     | 159  | THR  |
| 6   | H     | 162  | ASN  |
| 6   | H     | 164  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 171 | VAL  |
| 6   | H     | 173 | ILE  |
| 6   | H     | 179 | ASP  |
| 6   | H     | 188 | VAL  |
| 6   | H     | 197 | TRP  |
| 6   | H     | 199 | LEU  |
| 6   | H     | 243 | THR  |
| 6   | H     | 251 | ASN  |
| 6   | H     | 260 | ILE  |
| 6   | H     | 273 | MET  |
| 6   | H     | 287 | THR  |
| 6   | H     | 292 | ASN  |
| 6   | H     | 308 | TYR  |
| 6   | H     | 312 | GLN  |
| 6   | H     | 316 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1446 | GLN  |
| 4   | B     | 1494 | HIS  |
| 4   | B     | 1627 | GLN  |
| 4   | B     | 1634 | GLN  |
| 4   | B     | 1687 | HIS  |
| 4   | B     | 1693 | HIS  |
| 4   | B     | 1695 | GLN  |
| 4   | B     | 1703 | ASN  |
| 4   | B     | 1727 | GLN  |
| 4   | B     | 1758 | GLN  |
| 4   | B     | 1803 | HIS  |
| 4   | B     | 1958 | HIS  |
| 4   | B     | 1968 | HIS  |
| 4   | B     | 2082 | GLN  |
| 4   | B     | 2124 | GLN  |
| 4   | B     | 2154 | GLN  |
| 4   | B     | 2167 | GLN  |
| 4   | B     | 2178 | ASN  |
| 4   | B     | 2242 | HIS  |
| 4   | B     | 2277 | HIS  |
| 4   | B     | 2292 | ASN  |
| 4   | B     | 2385 | ASN  |
| 4   | B     | 2395 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 2410 | HIS  |
| 4   | B     | 2499 | GLN  |
| 4   | B     | 2531 | GLN  |
| 4   | B     | 2537 | ASN  |
| 4   | B     | 2540 | GLN  |
| 6   | D     | 28   | GLN  |
| 6   | D     | 40   | HIS  |
| 6   | D     | 74   | ASN  |
| 6   | D     | 132  | ASN  |
| 6   | D     | 140  | GLN  |
| 6   | D     | 153  | HIS  |
| 6   | D     | 161  | HIS  |
| 6   | D     | 162  | ASN  |
| 6   | D     | 164  | GLN  |
| 6   | D     | 209  | GLN  |
| 6   | D     | 312  | GLN  |
| 4   | F     | 1446 | GLN  |
| 4   | F     | 1494 | HIS  |
| 4   | F     | 1627 | GLN  |
| 4   | F     | 1634 | GLN  |
| 4   | F     | 1670 | HIS  |
| 4   | F     | 1687 | HIS  |
| 4   | F     | 1695 | GLN  |
| 4   | F     | 1727 | GLN  |
| 4   | F     | 1803 | HIS  |
| 4   | F     | 1941 | GLN  |
| 4   | F     | 1958 | HIS  |
| 4   | F     | 1968 | HIS  |
| 4   | F     | 1989 | ASN  |
| 4   | F     | 2082 | GLN  |
| 4   | F     | 2124 | GLN  |
| 4   | F     | 2167 | GLN  |
| 4   | F     | 2178 | ASN  |
| 4   | F     | 2277 | HIS  |
| 4   | F     | 2292 | ASN  |
| 4   | F     | 2385 | ASN  |
| 4   | F     | 2395 | ASN  |
| 4   | F     | 2410 | HIS  |
| 4   | F     | 2499 | GLN  |
| 4   | F     | 2531 | GLN  |
| 4   | F     | 2537 | ASN  |
| 4   | F     | 2540 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 28  | GLN  |
| 6   | H     | 74  | ASN  |
| 6   | H     | 132 | ASN  |
| 6   | H     | 140 | GLN  |
| 6   | H     | 153 | HIS  |
| 6   | H     | 161 | HIS  |
| 6   | H     | 162 | ASN  |
| 6   | H     | 164 | GLN  |
| 6   | H     | 209 | GLN  |
| 6   | H     | 312 | GLN  |

### 5.3.3 RNA [i](#)

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](#)

2 ligands are modelled in this entry.

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$ |
| 7   | RAP  | G     | 999 | -    | 65,68,68     | 1.32 | 6 (9%)      | 77,96,96    | 2.51 | 26 (33%)    |
| 7   | RAP  | C     | 999 | -    | 65,68,68     | 1.32 | 7 (10%)     | 77,96,96    | 2.52 | 25 (32%)    |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 7   | RAP  | G     | 999 | -    | 1/1/23/29 | 35/81/124/124 | 1/3/4/4 |
| 7   | RAP  | C     | 999 | -    | 1/1/23/29 | 36/81/124/124 | 1/3/4/4 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | G     | 999 | RAP  | O1-C1   | 4.42  | 1.44        | 1.34     |
| 7   | C     | 999 | RAP  | O1-C1   | 4.41  | 1.44        | 1.34     |
| 7   | C     | 999 | RAP  | C8-C9   | -4.40 | 1.47        | 1.53     |
| 7   | G     | 999 | RAP  | C8-C9   | -4.37 | 1.47        | 1.53     |
| 7   | C     | 999 | RAP  | O6-C10  | 3.39  | 1.44        | 1.39     |
| 7   | G     | 999 | RAP  | O6-C10  | 3.38  | 1.44        | 1.39     |
| 7   | C     | 999 | RAP  | C2-N7   | 2.77  | 1.50        | 1.47     |
| 7   | G     | 999 | RAP  | C2-N7   | 2.71  | 1.50        | 1.47     |
| 7   | C     | 999 | RAP  | C12-C11 | 2.13  | 1.56        | 1.53     |
| 7   | G     | 999 | RAP  | C12-C11 | 2.08  | 1.56        | 1.53     |
| 7   | C     | 999 | RAP  | C43-C11 | 2.04  | 1.57        | 1.53     |
| 7   | C     | 999 | RAP  | O1-C34  | -2.03 | 1.42        | 1.46     |
| 7   | G     | 999 | RAP  | O1-C34  | -2.02 | 1.42        | 1.46     |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | C     | 999 | RAP  | C28-C27-C26 | 6.99  | 121.16      | 111.25   |
| 7   | G     | 999 | RAP  | C28-C27-C26 | 6.86  | 120.98      | 111.25   |
| 7   | C     | 999 | RAP  | C48-C31-C30 | -6.42 | 104.58      | 110.73   |
| 7   | G     | 999 | RAP  | C48-C31-C30 | -6.40 | 104.59      | 110.73   |
| 7   | G     | 999 | RAP  | C14-C15-C16 | -6.22 | 100.43      | 114.49   |
| 7   | C     | 999 | RAP  | C14-C15-C16 | -6.19 | 100.49      | 114.49   |
| 7   | C     | 999 | RAP  | O4-C9-C8    | -5.54 | 112.84      | 119.08   |
| 7   | G     | 999 | RAP  | O4-C9-C8    | -5.51 | 112.88      | 119.08   |
| 7   | C     | 999 | RAP  | C43-C11-C12 | -5.36 | 102.51      | 110.33   |
| 7   | G     | 999 | RAP  | C43-C11-C12 | -5.35 | 102.53      | 110.33   |
| 7   | C     | 999 | RAP  | C12-C11-C10 | 5.27  | 117.09      | 110.28   |
| 7   | G     | 999 | RAP  | C12-C11-C10 | 5.22  | 117.03      | 110.28   |
| 7   | C     | 999 | RAP  | C47-C29-C28 | 5.04  | 126.62      | 115.85   |
| 7   | G     | 999 | RAP  | C47-C29-C28 | 5.04  | 126.61      | 115.85   |
| 7   | C     | 999 | RAP  | C27-C28-C29 | 4.73  | 124.88      | 112.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | G     | 999 | RAP  | C27-C28-C29 | 4.70  | 124.79      | 112.92   |
| 7   | C     | 999 | RAP  | C44-C17-C16 | 4.63  | 125.41      | 114.94   |
| 7   | G     | 999 | RAP  | C44-C17-C16 | 4.61  | 125.36      | 114.94   |
| 7   | G     | 999 | RAP  | C20-C19-C18 | -4.39 | 114.54      | 123.52   |
| 7   | C     | 999 | RAP  | C20-C19-C18 | -4.36 | 114.60      | 123.52   |
| 7   | G     | 999 | RAP  | C47-C29-C30 | -4.19 | 112.80      | 123.56   |
| 7   | C     | 999 | RAP  | C47-C29-C30 | -4.19 | 112.80      | 123.56   |
| 7   | G     | 999 | RAP  | O5-C14-C13  | 3.99  | 115.06      | 110.12   |
| 7   | C     | 999 | RAP  | O5-C14-C13  | 3.97  | 115.04      | 110.12   |
| 7   | C     | 999 | RAP  | C12-C13-C14 | -3.83 | 104.80      | 110.96   |
| 7   | G     | 999 | RAP  | C12-C13-C14 | -3.82 | 104.81      | 110.96   |
| 7   | G     | 999 | RAP  | O5-C14-C15  | 3.15  | 112.11      | 106.03   |
| 7   | C     | 999 | RAP  | O5-C14-C15  | 3.14  | 112.07      | 106.03   |
| 7   | C     | 999 | RAP  | C45-C23-C22 | -2.94 | 104.70      | 110.82   |
| 7   | G     | 999 | RAP  | C45-C23-C22 | -2.94 | 104.70      | 110.82   |
| 7   | C     | 999 | RAP  | C16-C17-C18 | -2.83 | 113.53      | 119.91   |
| 7   | G     | 999 | RAP  | C16-C17-C18 | -2.82 | 113.55      | 119.91   |
| 7   | G     | 999 | RAP  | O1-C1-C2    | 2.81  | 116.63      | 110.80   |
| 7   | C     | 999 | RAP  | O1-C1-C2    | 2.80  | 116.61      | 110.80   |
| 7   | C     | 999 | RAP  | C24-C23-C22 | 2.61  | 116.63      | 110.92   |
| 7   | G     | 999 | RAP  | C24-C23-C22 | 2.60  | 116.62      | 110.92   |
| 7   | G     | 999 | RAP  | C36-C35-C34 | 2.56  | 116.99      | 111.34   |
| 7   | C     | 999 | RAP  | C36-C35-C34 | 2.55  | 116.97      | 111.34   |
| 7   | G     | 999 | RAP  | C50-O7-C16  | 2.45  | 118.97      | 113.68   |
| 7   | C     | 999 | RAP  | C50-O7-C16  | 2.44  | 118.96      | 113.68   |
| 7   | G     | 999 | RAP  | C38-C39-C40 | -2.38 | 108.58      | 111.07   |
| 7   | C     | 999 | RAP  | C38-C39-C40 | -2.34 | 108.62      | 111.07   |
| 7   | C     | 999 | RAP  | C15-C16-C17 | 2.32  | 117.03      | 113.28   |
| 7   | G     | 999 | RAP  | C15-C16-C17 | 2.30  | 116.99      | 113.28   |
| 7   | G     | 999 | RAP  | O1-C1-O2    | -2.28 | 119.83      | 123.95   |
| 7   | C     | 999 | RAP  | O1-C1-O2    | -2.26 | 119.86      | 123.95   |
| 7   | G     | 999 | RAP  | C24-C25-C26 | 2.25  | 115.92      | 110.92   |
| 7   | C     | 999 | RAP  | C24-C25-C26 | 2.25  | 115.92      | 110.92   |
| 7   | C     | 999 | RAP  | C5-C4-C3    | -2.23 | 106.84      | 111.42   |
| 7   | G     | 999 | RAP  | C5-C4-C3    | -2.22 | 106.85      | 111.42   |
| 7   | G     | 999 | RAP  | C34-C33-C32 | 2.01  | 118.24      | 114.11   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 7   | C     | 999 | RAP  | C10  |
| 7   | G     | 999 | RAP  | C10  |

All (71) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | C     | 999 | RAP  | O3-C8-N7-C2     |
| 7   | C     | 999 | RAP  | O3-C8-N7-C6     |
| 7   | C     | 999 | RAP  | C9-C8-N7-C6     |
| 7   | C     | 999 | RAP  | O6-C10-C9-O4    |
| 7   | C     | 999 | RAP  | C15-C16-O7-C50  |
| 7   | C     | 999 | RAP  | C15-C16-C17-C18 |
| 7   | C     | 999 | RAP  | C15-C16-C17-C44 |
| 7   | C     | 999 | RAP  | C25-C26-C27-O9  |
| 7   | C     | 999 | RAP  | C26-C27-C28-O10 |
| 7   | C     | 999 | RAP  | C26-C27-C28-C29 |
| 7   | C     | 999 | RAP  | O9-C27-C28-O10  |
| 7   | C     | 999 | RAP  | O9-C27-C28-C29  |
| 7   | C     | 999 | RAP  | O10-C28-C29-C30 |
| 7   | C     | 999 | RAP  | O10-C28-C29-C47 |
| 7   | C     | 999 | RAP  | O1-C34-C35-C36  |
| 7   | C     | 999 | RAP  | C34-C35-C36-C37 |
| 7   | G     | 999 | RAP  | O3-C8-N7-C2     |
| 7   | G     | 999 | RAP  | O3-C8-N7-C6     |
| 7   | G     | 999 | RAP  | C9-C8-N7-C6     |
| 7   | G     | 999 | RAP  | O6-C10-C9-O4    |
| 7   | G     | 999 | RAP  | C15-C16-O7-C50  |
| 7   | G     | 999 | RAP  | C15-C16-C17-C18 |
| 7   | G     | 999 | RAP  | C15-C16-C17-C44 |
| 7   | G     | 999 | RAP  | C25-C26-C27-O9  |
| 7   | G     | 999 | RAP  | C26-C27-C28-O10 |
| 7   | G     | 999 | RAP  | C26-C27-C28-C29 |
| 7   | G     | 999 | RAP  | O9-C27-C28-O10  |
| 7   | G     | 999 | RAP  | O9-C27-C28-C29  |
| 7   | G     | 999 | RAP  | O10-C28-C29-C30 |
| 7   | G     | 999 | RAP  | O10-C28-C29-C47 |
| 7   | G     | 999 | RAP  | O1-C34-C35-C36  |
| 7   | G     | 999 | RAP  | C34-C35-C36-C37 |
| 7   | C     | 999 | RAP  | C17-C18-C19-C20 |
| 7   | G     | 999 | RAP  | C17-C18-C19-C20 |
| 7   | C     | 999 | RAP  | C19-C20-C21-C22 |
| 7   | G     | 999 | RAP  | C19-C20-C21-C22 |
| 7   | C     | 999 | RAP  | C28-C29-C30-C31 |
| 7   | G     | 999 | RAP  | C28-C29-C30-C31 |
| 7   | C     | 999 | RAP  | C23-C24-C25-C26 |
| 7   | G     | 999 | RAP  | C23-C24-C25-C26 |
| 7   | C     | 999 | RAP  | C46-C25-C26-O8  |
| 7   | G     | 999 | RAP  | C46-C25-C26-O8  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | C     | 999 | RAP  | C46-C25-C26-C27 |
| 7   | C     | 999 | RAP  | C47-C29-C30-C31 |
| 7   | G     | 999 | RAP  | C46-C25-C26-C27 |
| 7   | G     | 999 | RAP  | C47-C29-C30-C31 |
| 7   | C     | 999 | RAP  | C23-C24-C25-C46 |
| 7   | G     | 999 | RAP  | C23-C24-C25-C46 |
| 7   | C     | 999 | RAP  | C2-C1-O1-C34    |
| 7   | G     | 999 | RAP  | C2-C1-O1-C34    |
| 7   | C     | 999 | RAP  | C35-C36-C37-C38 |
| 7   | G     | 999 | RAP  | C35-C36-C37-C38 |
| 7   | C     | 999 | RAP  | O8-C26-C27-C28  |
| 7   | G     | 999 | RAP  | O2-C1-O1-C34    |
| 7   | C     | 999 | RAP  | C49-C35-C36-C37 |
| 7   | G     | 999 | RAP  | C49-C35-C36-C37 |
| 7   | C     | 999 | RAP  | O2-C1-O1-C34    |
| 7   | C     | 999 | RAP  | C25-C26-C27-C28 |
| 7   | G     | 999 | RAP  | C25-C26-C27-C28 |
| 7   | C     | 999 | RAP  | C9-C8-N7-C2     |
| 7   | G     | 999 | RAP  | C9-C8-N7-C2     |
| 7   | C     | 999 | RAP  | O8-C26-C27-O9   |
| 7   | G     | 999 | RAP  | O8-C26-C27-O9   |
| 7   | C     | 999 | RAP  | C11-C10-C9-O4   |
| 7   | G     | 999 | RAP  | C11-C10-C9-O4   |
| 7   | C     | 999 | RAP  | C38-C39-O12-C52 |
| 7   | C     | 999 | RAP  | C35-C36-C37-C42 |
| 7   | G     | 999 | RAP  | C35-C36-C37-C42 |
| 7   | G     | 999 | RAP  | C38-C39-O12-C52 |
| 7   | C     | 999 | RAP  | C33-C34-C35-C36 |
| 7   | G     | 999 | RAP  | C33-C34-C35-C36 |

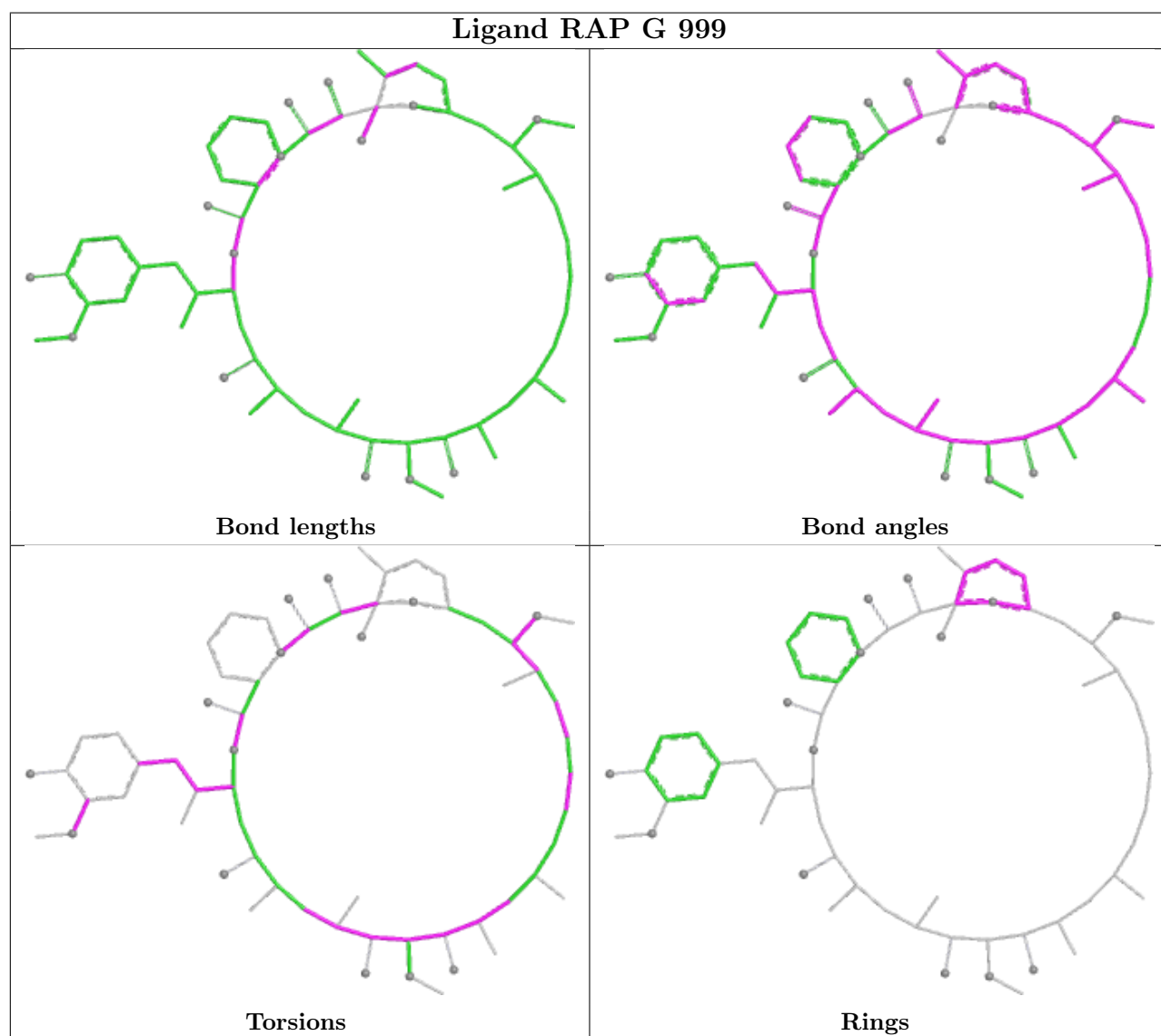
All (2) ring outliers are listed below:

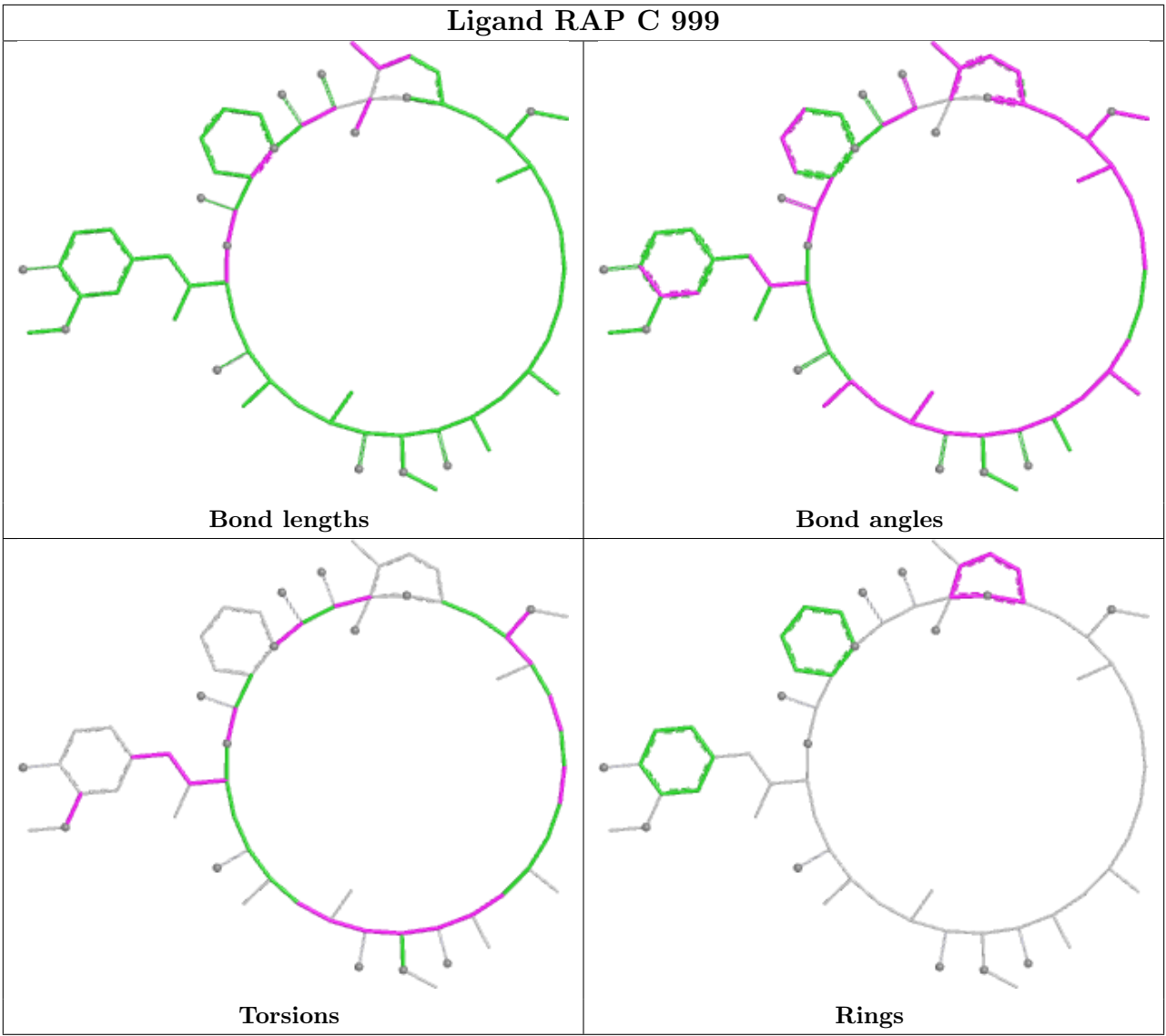
| Mol | Chain | Res | Type | Atoms                  |
|-----|-------|-----|------|------------------------|
| 7   | G     | 999 | RAP  | C10-C11-C12-C13-C14-O5 |
| 7   | C     | 999 | RAP  | C10-C11-C12-C13-C14-O5 |

2 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | G     | 999 | RAP  | 4       | 0            |
| 7   | C     | 999 | RAP  | 6       | 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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 1     | 23               |
| 1   | 3     | 23               |
| 3   | A     | 11               |
| 3   | E     | 11               |
| 2   | 2     | 5                |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | 4     | 5                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1221:UNK  | C      | 1300:UNK  | N      | 39.71        |
| 1     | E     | 1221:UNK  | C      | 1300:UNK  | N      | 39.71        |
| 1     | 2     | 271:UNK   | C      | 300:UNK   | N      | 29.88        |
| 1     | 4     | 271:UNK   | C      | 300:UNK   | N      | 29.87        |
| 1     | A     | 1152:UNK  | C      | 1200:UNK  | N      | 25.69        |
| 1     | E     | 1152:UNK  | C      | 1200:UNK  | N      | 25.69        |
| 1     | E     | 1000:UNK  | C      | 1100:UNK  | N      | 19.99        |
| 1     | A     | 1000:UNK  | C      | 1100:UNK  | N      | 19.98        |
| 1     | E     | 431:UNK   | C      | 500:UNK   | N      | 19.29        |
| 1     | A     | 431:UNK   | C      | 500:UNK   | N      | 19.28        |
| 1     | A     | 1417:UNK  | C      | 1500:UNK  | N      | 15.10        |
| 1     | E     | 1417:UNK  | C      | 1500:UNK  | N      | 15.10        |
| 1     | 1     | 715:UNK   | C      | 800:UNK   | N      | 15.00        |
| 1     | 3     | 715:UNK   | C      | 800:UNK   | N      | 14.99        |
| 1     | 3     | 457:UNK   | C      | 500:UNK   | N      | 14.45        |
| 1     | 1     | 457:UNK   | C      | 500:UNK   | N      | 14.44        |
| 1     | A     | 334:UNK   | C      | 400:UNK   | N      | 14.26        |
| 1     | E     | 334:UNK   | C      | 400:UNK   | N      | 14.25        |
| 1     | A     | 124:UNK   | C      | 200:UNK   | N      | 13.44        |
| 1     | E     | 124:UNK   | C      | 200:UNK   | N      | 13.43        |
| 1     | 3     | 1114:UNK  | C      | 1200:UNK  | N      | 11.96        |
| 1     | 1     | 1114:UNK  | C      | 1200:UNK  | N      | 11.95        |
| 1     | 2     | 556:UNK   | C      | 600:UNK   | N      | 11.85        |
| 1     | 4     | 556:UNK   | C      | 600:UNK   | N      | 11.85        |
| 1     | 1     | 1412:UNK  | C      | 1500:UNK  | N      | 11.83        |
| 1     | 3     | 1412:UNK  | C      | 1500:UNK  | N      | 11.83        |
| 1     | 1     | 1616:UNK  | C      | 1700:UNK  | N      | 11.09        |
| 1     | 3     | 1616:UNK  | C      | 1700:UNK  | N      | 11.09        |
| 1     | A     | 1668:UNK  | C      | 1700:UNK  | N      | 10.21        |
| 1     | E     | 1668:UNK  | C      | 1700:UNK  | N      | 10.20        |
| 1     | 1     | 1813:UNK  | C      | 1900:UNK  | N      | 10.04        |
| 1     | 3     | 1813:UNK  | C      | 1900:UNK  | N      | 10.03        |
| 1     | 1     | 815:UNK   | C      | 900:UNK   | N      | 9.88         |
| 1     | 3     | 815:UNK   | C      | 900:UNK   | N      | 9.88         |
| 1     | 1     | 1315:UNK  | C      | 1400:UNK  | N      | 9.83         |
| 1     | 3     | 1315:UNK  | C      | 1400:UNK  | N      | 9.83         |
| 1     | 1     | 1030:UNK  | C      | 1100:UNK  | N      | 9.70         |
| 1     | 3     | 1030:UNK  | C      | 1100:UNK  | N      | 9.70         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 259:UNK   | C      | 300:UNK   | N      | 9.60         |
| 1     | E     | 259:UNK   | C      | 300:UNK   | N      | 9.59         |
| 1     | 4     | 310:UNK   | C      | 400:UNK   | N      | 8.54         |
| 1     | 2     | 310:UNK   | C      | 400:UNK   | N      | 8.52         |
| 1     | 1     | 616:UNK   | C      | 700:UNK   | N      | 8.41         |
| 1     | 3     | 616:UNK   | C      | 700:UNK   | N      | 8.40         |
| 1     | 1     | 2016:UNK  | C      | 2100:UNK  | N      | 8.19         |
| 1     | 3     | 2016:UNK  | C      | 2100:UNK  | N      | 8.19         |
| 1     | 3     | 513:UNK   | C      | 600:UNK   | N      | 8.16         |
| 1     | 1     | 513:UNK   | C      | 600:UNK   | N      | 8.15         |
| 1     | 3     | 1718:UNK  | C      | 1800:UNK  | N      | 8.07         |
| 1     | 1     | 1718:UNK  | C      | 1800:UNK  | N      | 8.06         |
| 1     | 3     | 933:UNK   | C      | 1000:UNK  | N      | 6.84         |
| 1     | 1     | 933:UNK   | C      | 1000:UNK  | N      | 6.83         |
| 1     | 1     | 1219:UNK  | C      | 1300:UNK  | N      | 6.81         |
| 1     | 3     | 1219:UNK  | C      | 1300:UNK  | N      | 6.80         |
| 1     | 3     | 2220:UNK  | C      | 2300:UNK  | N      | 6.69         |
| 1     | 1     | 2220:UNK  | C      | 2300:UNK  | N      | 6.68         |
| 1     | E     | 655:UNK   | C      | 700:UNK   | N      | 6.29         |
| 1     | 1     | 2117:UNK  | C      | 2200:UNK  | N      | 6.28         |
| 1     | 3     | 2117:UNK  | C      | 2200:UNK  | N      | 6.28         |
| 1     | A     | 655:UNK   | C      | 700:UNK   | N      | 6.26         |
| 1     | 3     | 1014:UNK  | C      | 1015:UNK  | N      | 6.17         |
| 1     | 1     | 1014:UNK  | C      | 1015:UNK  | N      | 6.16         |
| 1     | 3     | 1516:UNK  | C      | 1600:UNK  | N      | 6.12         |
| 1     | 1     | 1516:UNK  | C      | 1600:UNK  | N      | 6.11         |
| 1     | 1     | 335:UNK   | C      | 400:UNK   | N      | 5.34         |
| 1     | 3     | 335:UNK   | C      | 400:UNK   | N      | 5.34         |
| 1     | 4     | 408:UNK   | C      | 500:UNK   | N      | 5.10         |
| 1     | 2     | 408:UNK   | C      | 500:UNK   | N      | 5.09         |
| 1     | E     | 24:UNK    | C      | 100:UNK   | N      | 4.74         |
| 1     | A     | 24:UNK    | C      | 100:UNK   | N      | 4.73         |
| 1     | 4     | 197:UNK   | C      | 200:UNK   | N      | 4.05         |
| 1     | 2     | 197:UNK   | C      | 200:UNK   | N      | 4.03         |
| 1     | 1     | 160:UNK   | C      | 200:UNK   | N      | 3.81         |
| 1     | 3     | 160:UNK   | C      | 200:UNK   | N      | 3.78         |
| 1     | 3     | 1916:UNK  | C      | 2000:UNK  | N      | 3.51         |
| 1     | 1     | 1916:UNK  | C      | 2000:UNK  | N      | 3.50         |
| 1     | 1     | 214:UNK   | C      | 300:UNK   | N      | 3.11         |
| 1     | 3     | 214:UNK   | C      | 300:UNK   | N      | 3.10         |

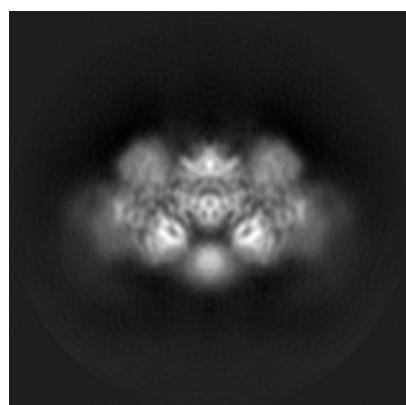
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3213. These allow visual inspection of the internal detail of the map and identification of artifacts.

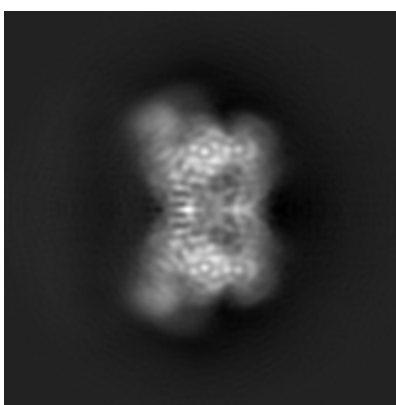
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

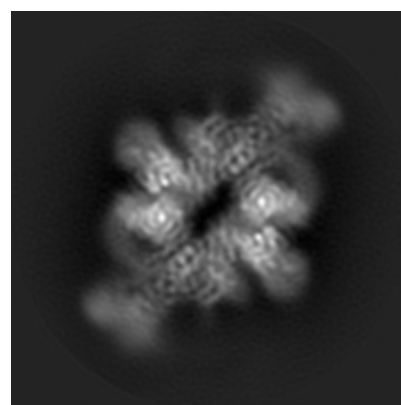
#### 6.1.1 Primary map



X



Y

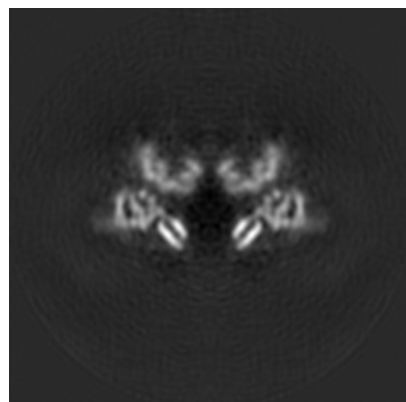


Z

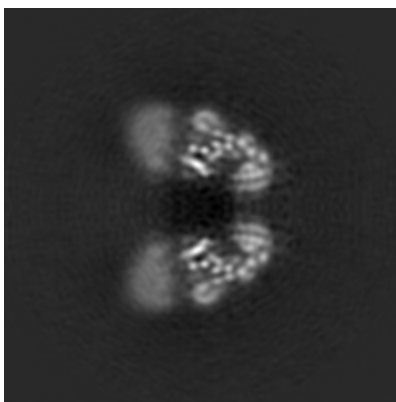
The images above show the map projected in three orthogonal directions.

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

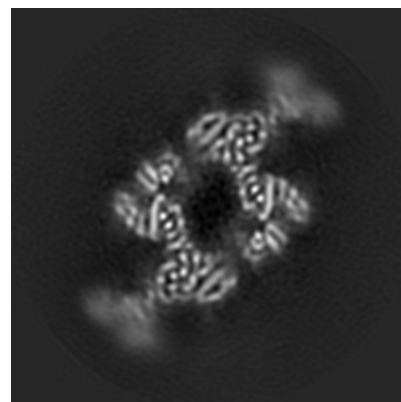
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

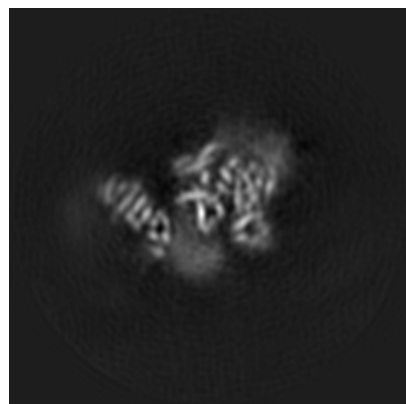


Z Index: 128

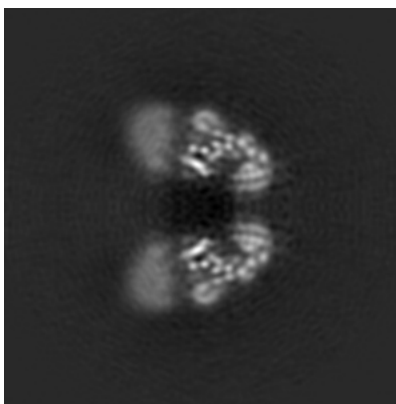
The images above show central slices of the map in three orthogonal directions.

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

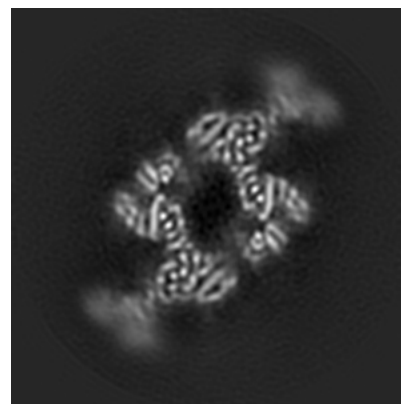
### 6.3.1 Primary map



X Index: 96



Y Index: 128

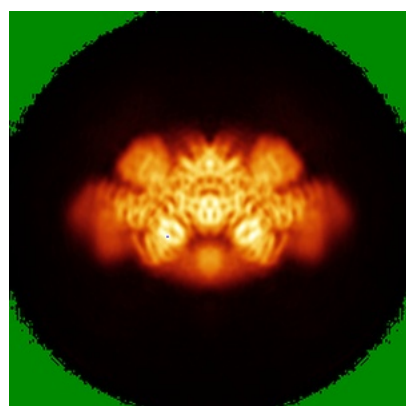


Z Index: 128

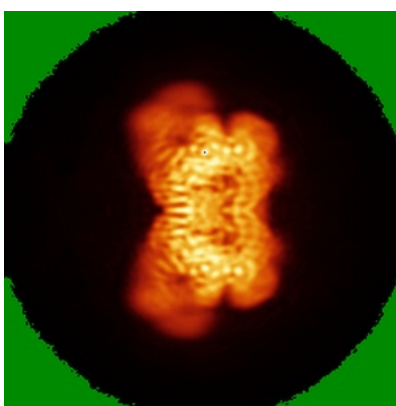
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

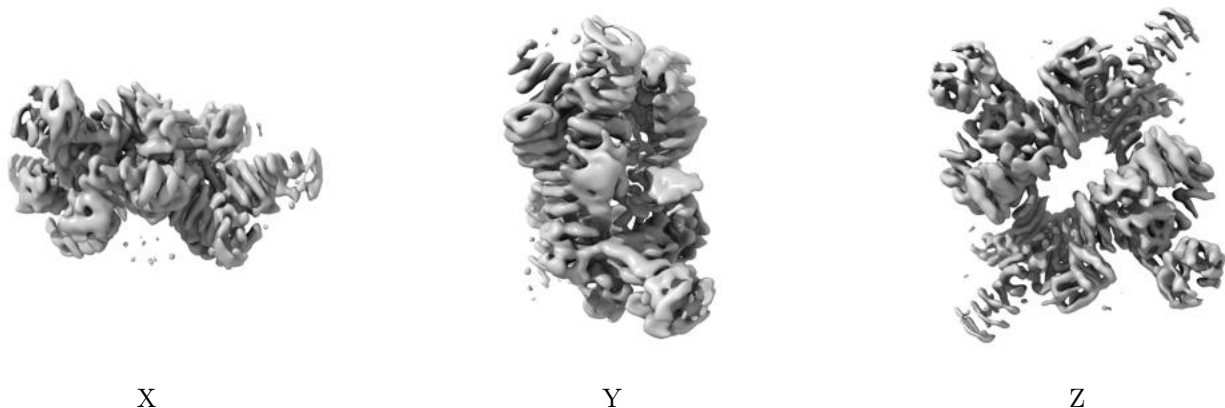


Z

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 0.066. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

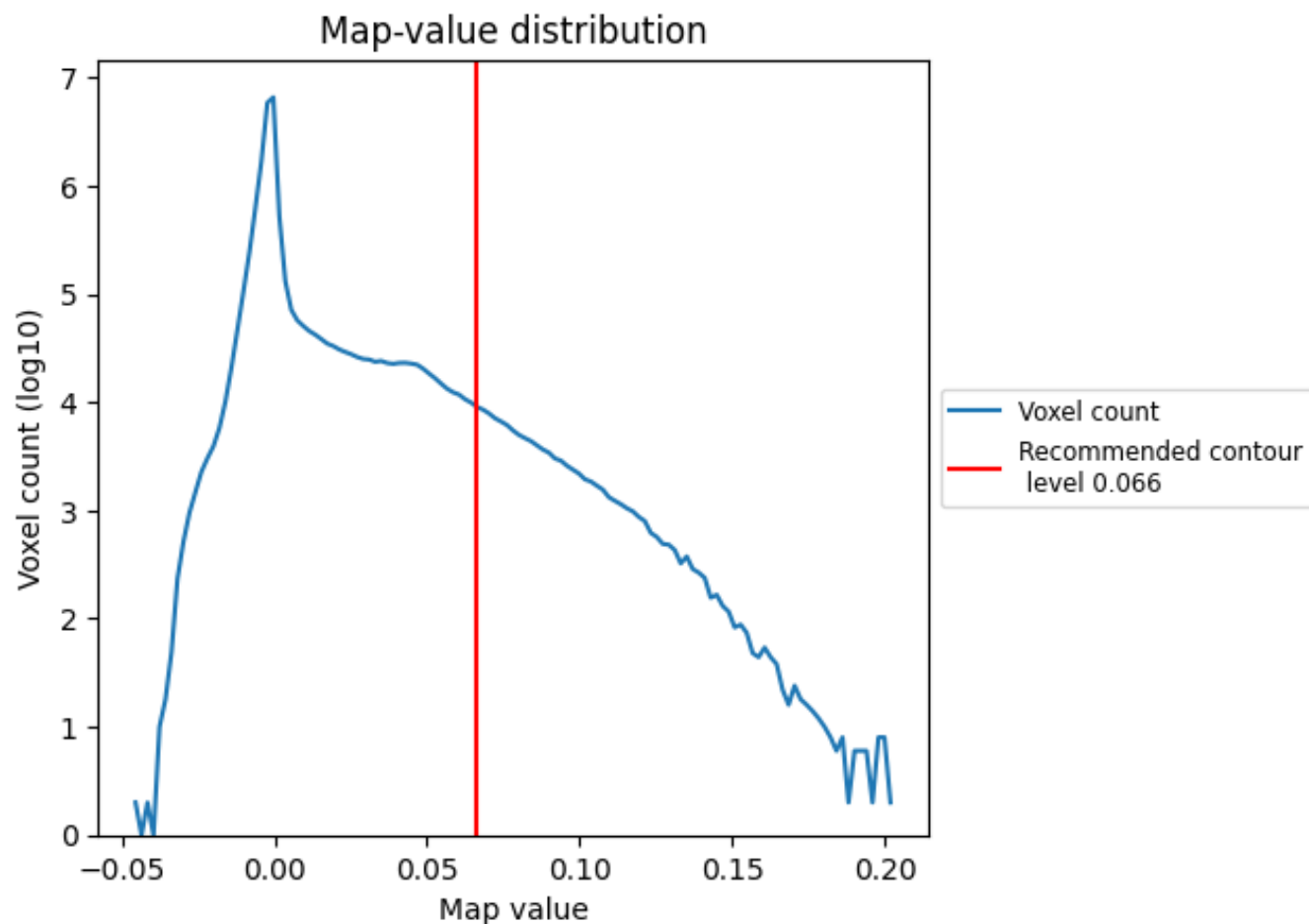
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

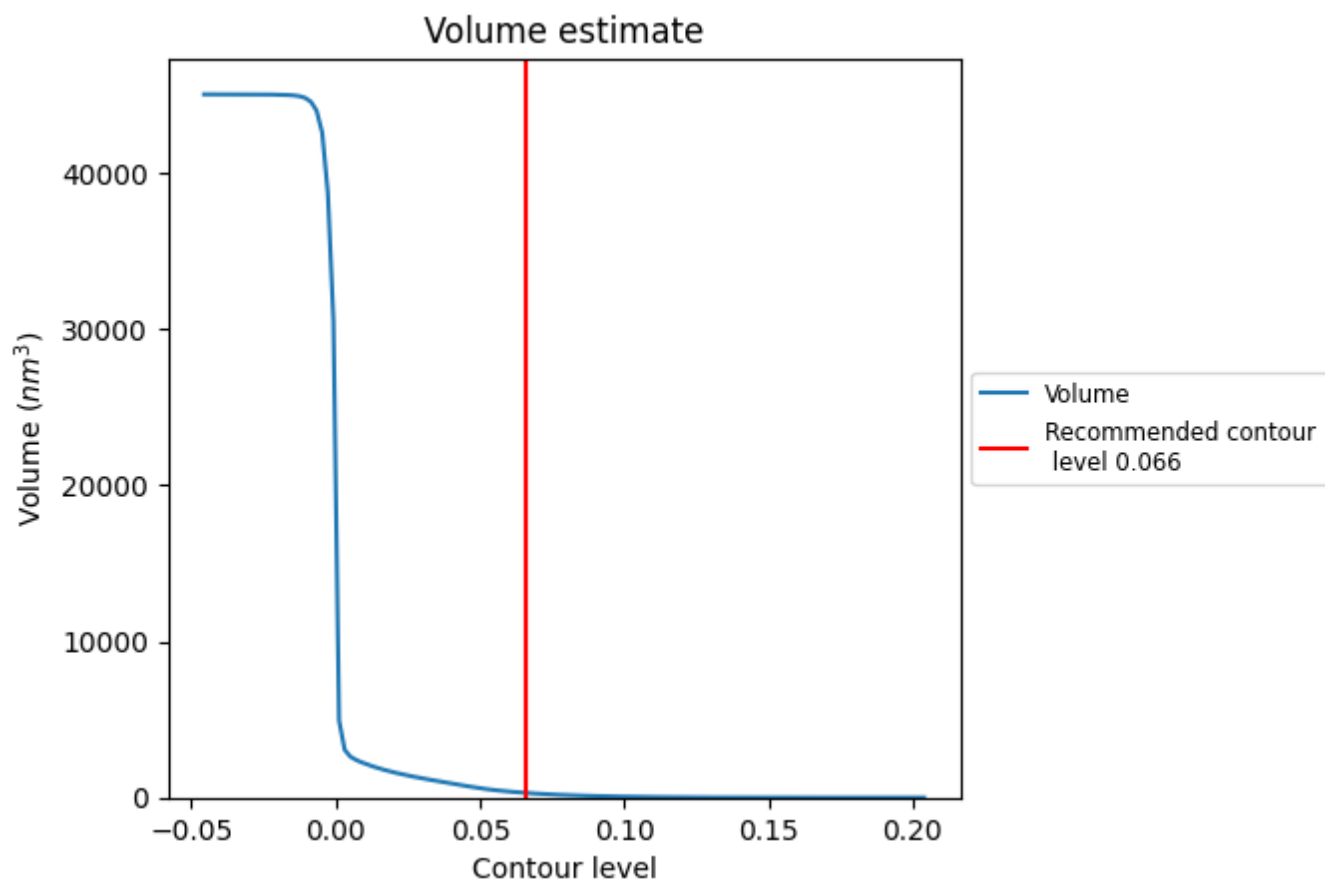
This section contains the results of statistical analysis of the map.

### 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.

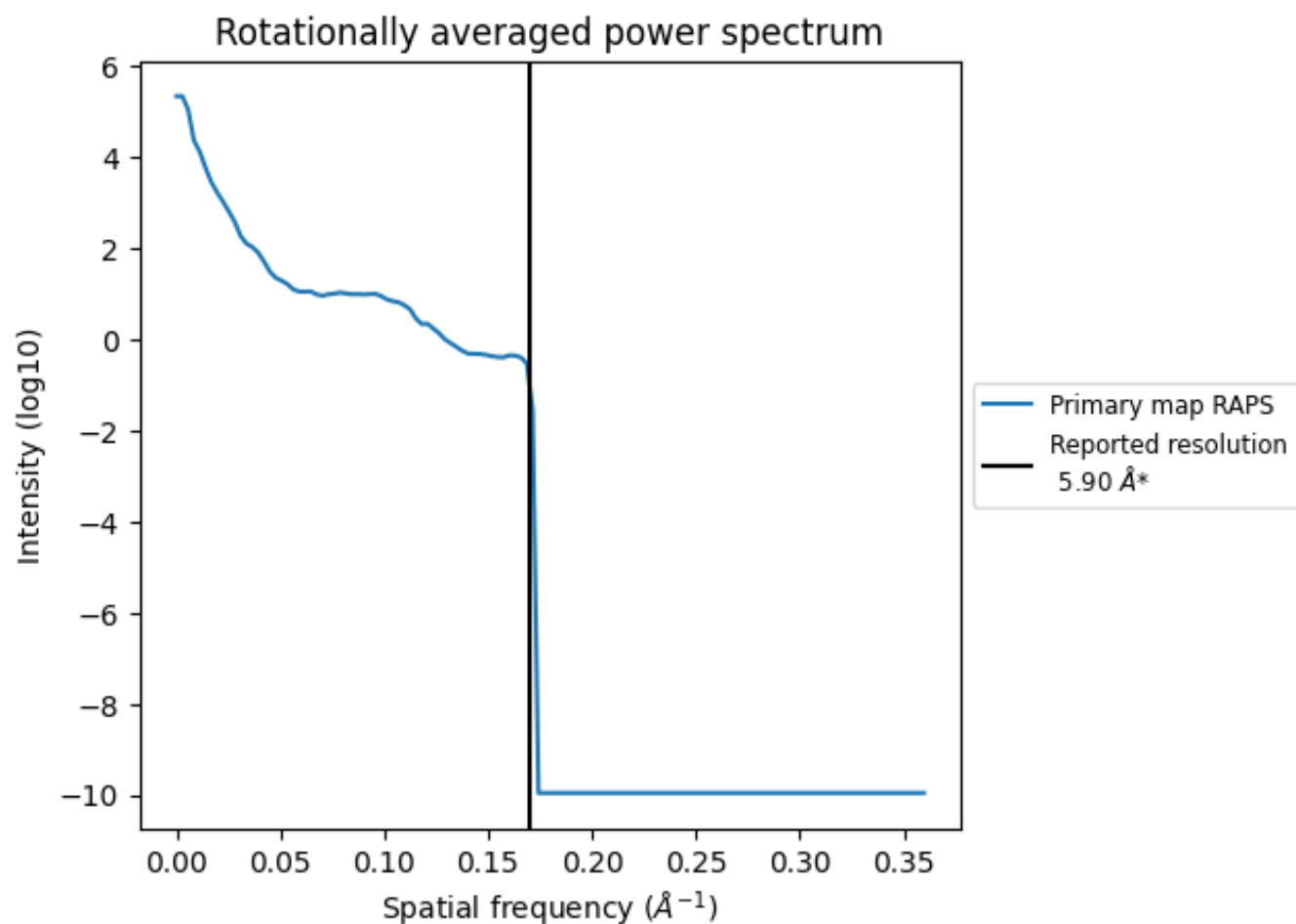
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm<sup>3</sup>; this corresponds to an approximate mass of 269 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 0.169  $\text{\AA}^{-1}$

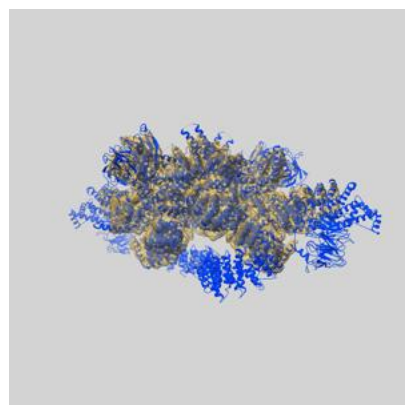
## 8 Fourier-Shell correlation ⓘ

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

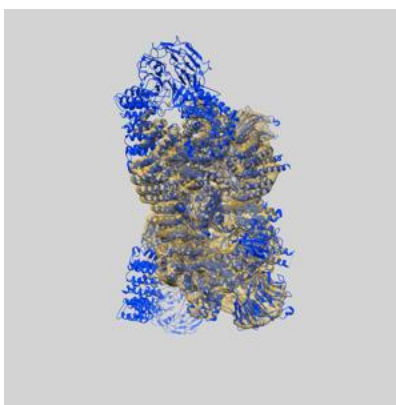
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3213 and PDB model 5FLC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

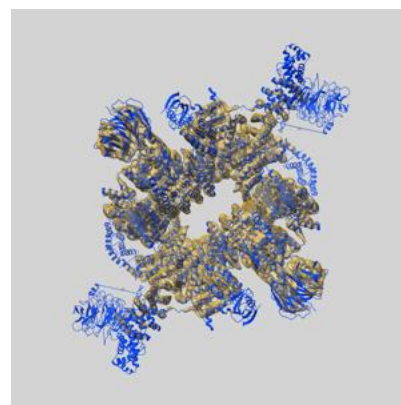
### 9.1 Map-model overlay [i](#)



X



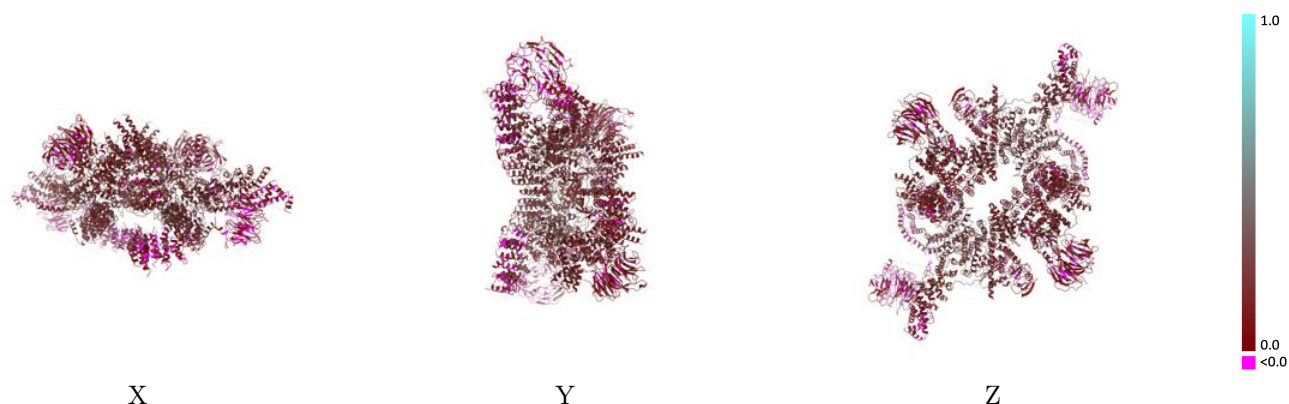
Y



Z

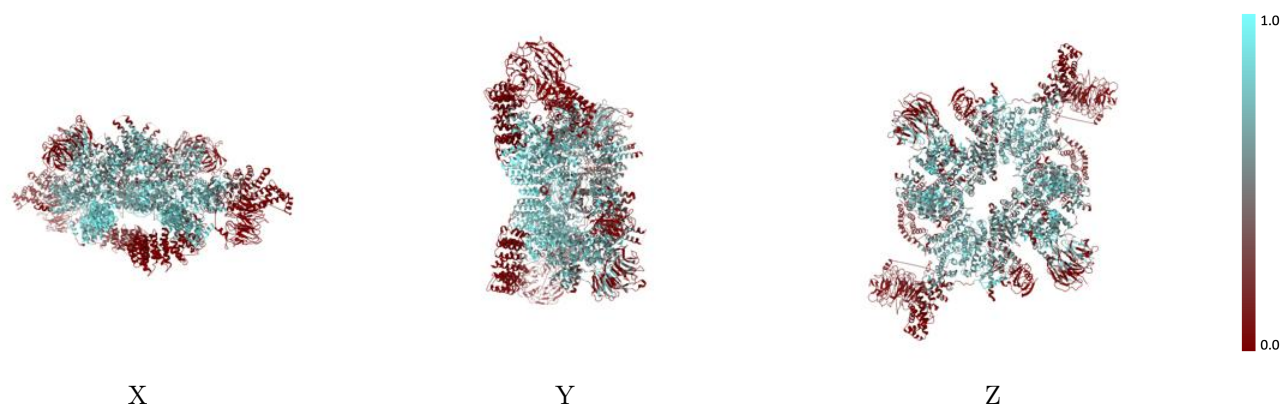
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



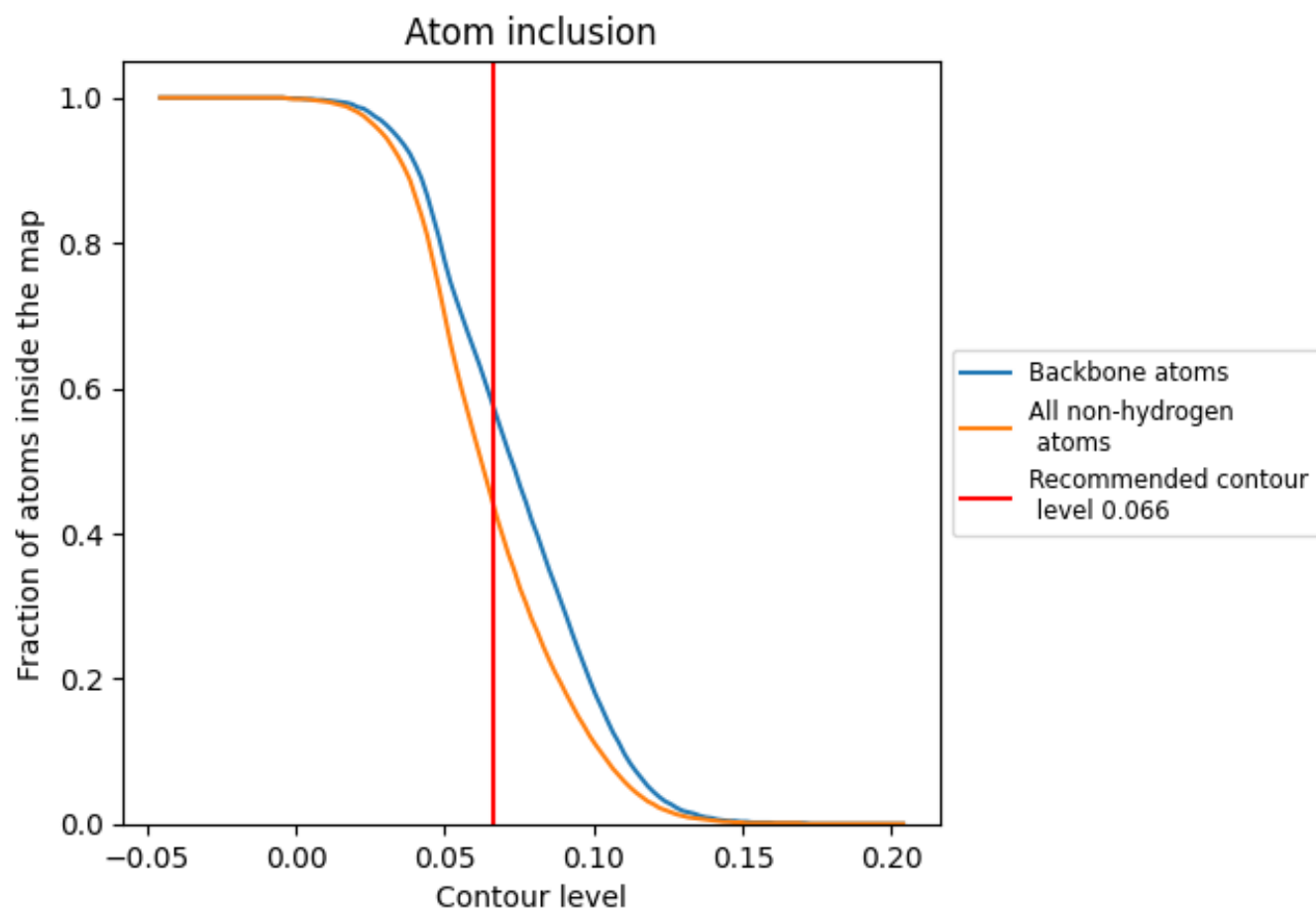
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.066).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 44% 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 (0.066) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4430 | <div></div> 0.1700 |
| 1     | <div></div> 0.3450 | <div></div> 0.1590 |
| 2     | <div></div> 0.8130 | <div></div> 0.2430 |
| 3     | <div></div> 0.3450 | <div></div> 0.1590 |
| 4     | <div></div> 0.8130 | <div></div> 0.2440 |
| A     | <div></div> 0.2890 | <div></div> 0.1580 |
| B     | <div></div> 0.5790 | <div></div> 0.1810 |
| C     | <div></div> 0.0070 | <div></div> 0.1250 |
| D     | <div></div> 0.3100 | <div></div> 0.1240 |
| E     | <div></div> 0.2890 | <div></div> 0.1580 |
| F     | <div></div> 0.5780 | <div></div> 0.1810 |
| G     | <div></div> 0.0070 | <div></div> 0.1340 |
| H     | <div></div> 0.3100 | <div></div> 0.1250 |

1.0

0.0

<0.0