



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:32 AM UTC

PDB ID : 6C3O / pdb\_00006c3o  
EMDB ID : EMD-7338  
Title : Cryo-EM structure of human KATP bound to ATP and ADP in quatrefoil form  
Authors : Lee, K.P.K.; Chen, J.; MacKinnon, R.  
Deposited on : 2018-01-10  
Resolution : 3.90 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:

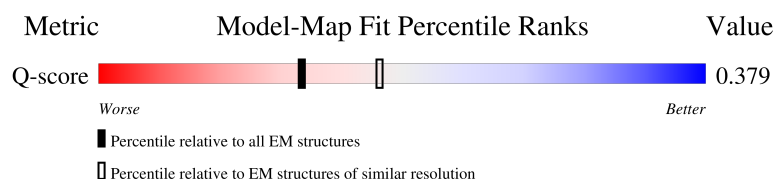
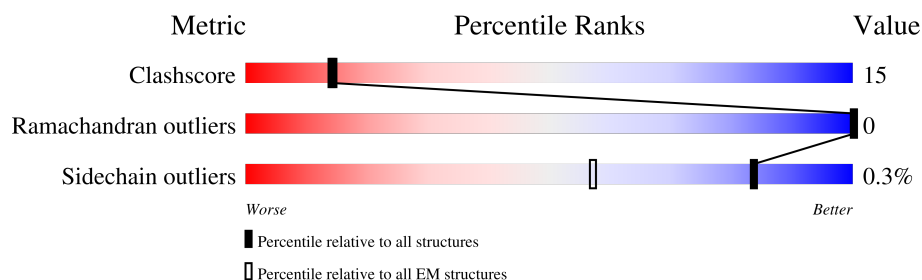
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.90 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.



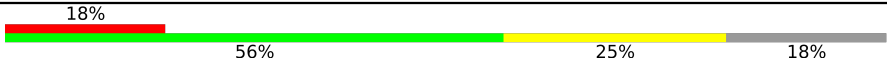
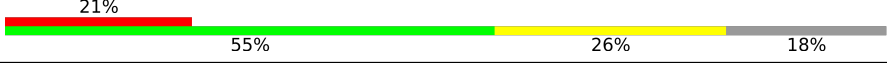
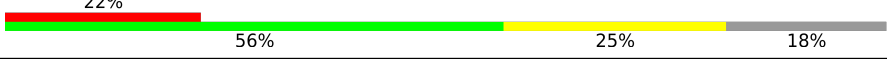
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8855 ( 3.40 - 4.40 )                                     |

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   | A     | 406    | <div> <div>12%</div> <div>50%</div> <div>30%</div> <div>19%</div> </div> |
| 1   | B     | 406    | <div> <div>12%</div> <div>49%</div> <div>32%</div> <div>19%</div> </div> |
| 1   | C     | 406    | <div> <div>14%</div> <div>50%</div> <div>31%</div> <div>19%</div> </div> |
| 1   | D     | 406    | <div> <div>14%</div> <div>49%</div> <div>32%</div> <div>19%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | E     | 1581   |  |
| 2   | F     | 1581   |  |
| 2   | G     | 1581   |  |
| 2   | H     | 1581   |  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49055 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 ATP-sensitive inward rectifier potassium channel 11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2501  | 1616 | 427 | 441 | 17 |         |       |
| 1   | C     | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2501  | 1616 | 427 | 441 | 17 |         |       |
| 1   | B     | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2501  | 1616 | 427 | 441 | 17 |         |       |
| 1   | D     | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2501  | 1616 | 427 | 441 | 17 |         |       |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -5      | SER      | -      | expression tag | UNP Q14654 |
| A     | -4      | ALA      | -      | expression tag | UNP Q14654 |
| A     | -3      | SER      | -      | expression tag | UNP Q14654 |
| A     | -2      | ALA      | -      | expression tag | UNP Q14654 |
| A     | -1      | SER      | -      | expression tag | UNP Q14654 |
| A     | 0       | ALA      | -      | expression tag | UNP Q14654 |
| A     | 391     | SER      | -      | expression tag | UNP Q14654 |
| A     | 392     | ASN      | -      | expression tag | UNP Q14654 |
| A     | 393     | SER      | -      | expression tag | UNP Q14654 |
| A     | 394     | LEU      | -      | expression tag | UNP Q14654 |
| A     | 395     | GLU      | -      | expression tag | UNP Q14654 |
| A     | 396     | VAL      | -      | expression tag | UNP Q14654 |
| A     | 397     | LEU      | -      | expression tag | UNP Q14654 |
| A     | 398     | PHE      | -      | expression tag | UNP Q14654 |
| A     | 399     | GLN      | -      | expression tag | UNP Q14654 |
| A     | 400     | GLY      | -      | expression tag | UNP Q14654 |
| C     | -5      | SER      | -      | expression tag | UNP Q14654 |
| C     | -4      | ALA      | -      | expression tag | UNP Q14654 |
| C     | -3      | SER      | -      | expression tag | UNP Q14654 |
| C     | -2      | ALA      | -      | expression tag | UNP Q14654 |
| C     | -1      | SER      | -      | expression tag | UNP Q14654 |
| C     | 0       | ALA      | -      | expression tag | UNP Q14654 |

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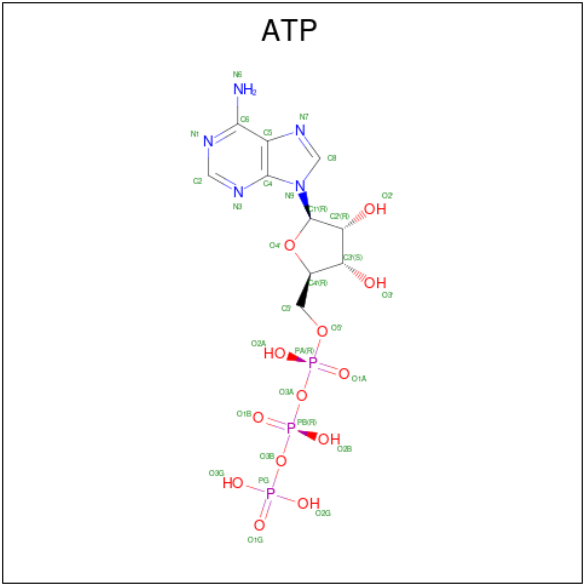
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 391     | SER      | -      | expression tag | UNP Q14654 |
| C     | 392     | ASN      | -      | expression tag | UNP Q14654 |
| C     | 393     | SER      | -      | expression tag | UNP Q14654 |
| C     | 394     | LEU      | -      | expression tag | UNP Q14654 |
| C     | 395     | GLU      | -      | expression tag | UNP Q14654 |
| C     | 396     | VAL      | -      | expression tag | UNP Q14654 |
| C     | 397     | LEU      | -      | expression tag | UNP Q14654 |
| C     | 398     | PHE      | -      | expression tag | UNP Q14654 |
| C     | 399     | GLN      | -      | expression tag | UNP Q14654 |
| C     | 400     | GLY      | -      | expression tag | UNP Q14654 |
| B     | -5      | SER      | -      | expression tag | UNP Q14654 |
| B     | -4      | ALA      | -      | expression tag | UNP Q14654 |
| B     | -3      | SER      | -      | expression tag | UNP Q14654 |
| B     | -2      | ALA      | -      | expression tag | UNP Q14654 |
| B     | -1      | SER      | -      | expression tag | UNP Q14654 |
| B     | 0       | ALA      | -      | expression tag | UNP Q14654 |
| B     | 391     | SER      | -      | expression tag | UNP Q14654 |
| B     | 392     | ASN      | -      | expression tag | UNP Q14654 |
| B     | 393     | SER      | -      | expression tag | UNP Q14654 |
| B     | 394     | LEU      | -      | expression tag | UNP Q14654 |
| B     | 395     | GLU      | -      | expression tag | UNP Q14654 |
| B     | 396     | VAL      | -      | expression tag | UNP Q14654 |
| B     | 397     | LEU      | -      | expression tag | UNP Q14654 |
| B     | 398     | PHE      | -      | expression tag | UNP Q14654 |
| B     | 399     | GLN      | -      | expression tag | UNP Q14654 |
| B     | 400     | GLY      | -      | expression tag | UNP Q14654 |
| D     | -5      | SER      | -      | expression tag | UNP Q14654 |
| D     | -4      | ALA      | -      | expression tag | UNP Q14654 |
| D     | -3      | SER      | -      | expression tag | UNP Q14654 |
| D     | -2      | ALA      | -      | expression tag | UNP Q14654 |
| D     | -1      | SER      | -      | expression tag | UNP Q14654 |
| D     | 0       | ALA      | -      | expression tag | UNP Q14654 |
| D     | 391     | SER      | -      | expression tag | UNP Q14654 |
| D     | 392     | ASN      | -      | expression tag | UNP Q14654 |
| D     | 393     | SER      | -      | expression tag | UNP Q14654 |
| D     | 394     | LEU      | -      | expression tag | UNP Q14654 |
| D     | 395     | GLU      | -      | expression tag | UNP Q14654 |
| D     | 396     | VAL      | -      | expression tag | UNP Q14654 |
| D     | 397     | LEU      | -      | expression tag | UNP Q14654 |
| D     | 398     | PHE      | -      | expression tag | UNP Q14654 |
| D     | 399     | GLN      | -      | expression tag | UNP Q14654 |
| D     | 400     | GLY      | -      | expression tag | UNP Q14654 |

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | E     | 1290     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9671  | 6307 | 1626 | 1687 | 51 |         |       |
| 2   | H     | 1290     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9671  | 6307 | 1626 | 1687 | 51 |         |       |
| 2   | G     | 1290     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9671  | 6307 | 1626 | 1687 | 51 |         |       |
| 2   | F     | 1290     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9671  | 6307 | 1626 | 1687 | 51 |         |       |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

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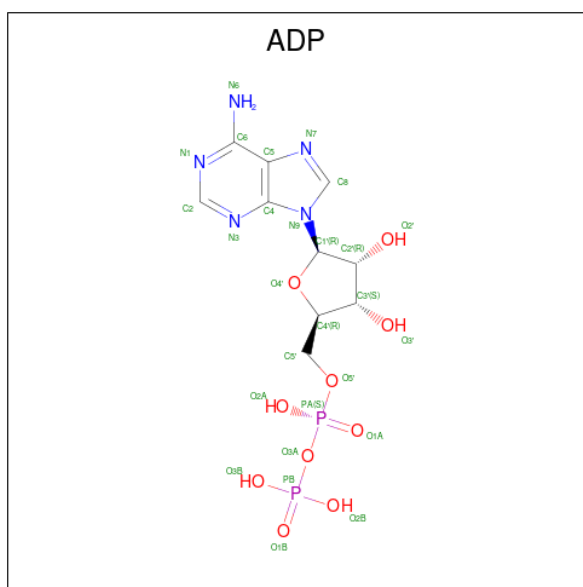
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 4   | A     | 3        | Total | K | 0       |
|     |       |          | 3     | 3 |         |

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 5   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 5   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 5   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | E     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

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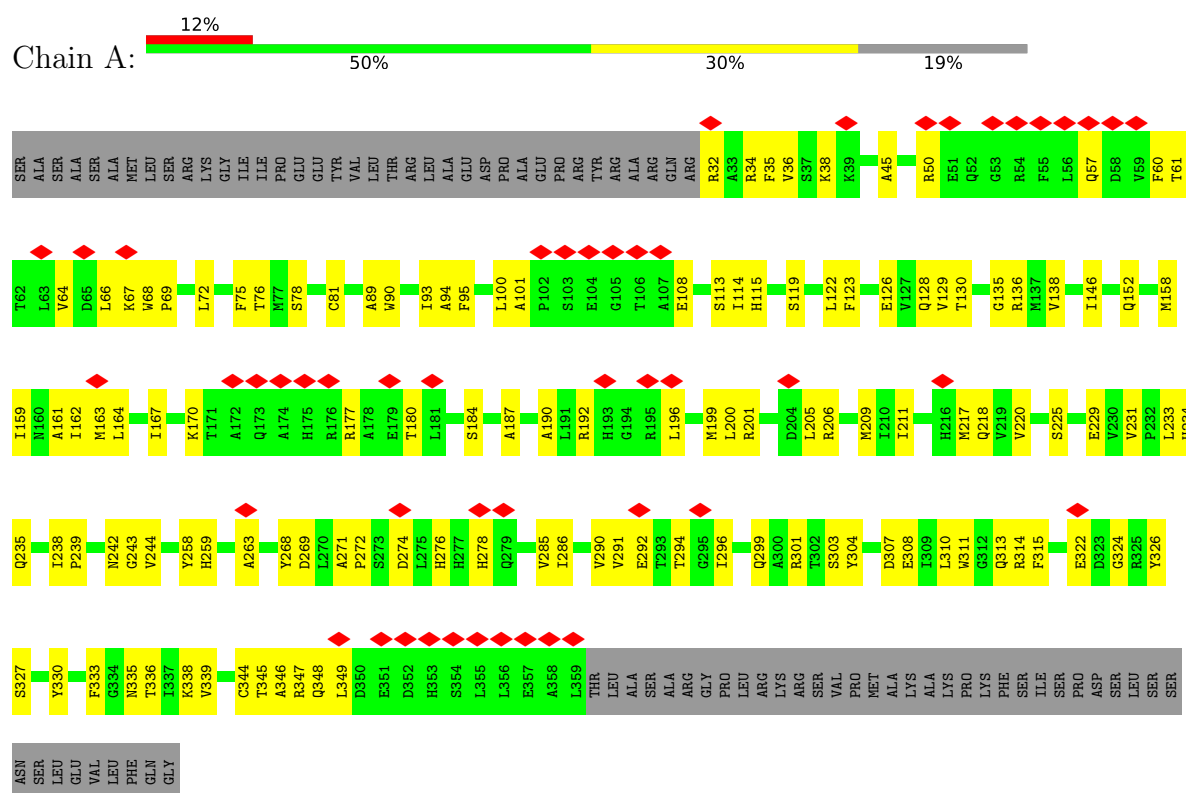
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 6   | H     | 2        | Total<br>2 | Mg<br>2 | 0       |
| 6   | G     | 2        | Total<br>2 | Mg<br>2 | 0       |
| 6   | F     | 2        | Total<br>2 | Mg<br>2 | 0       |



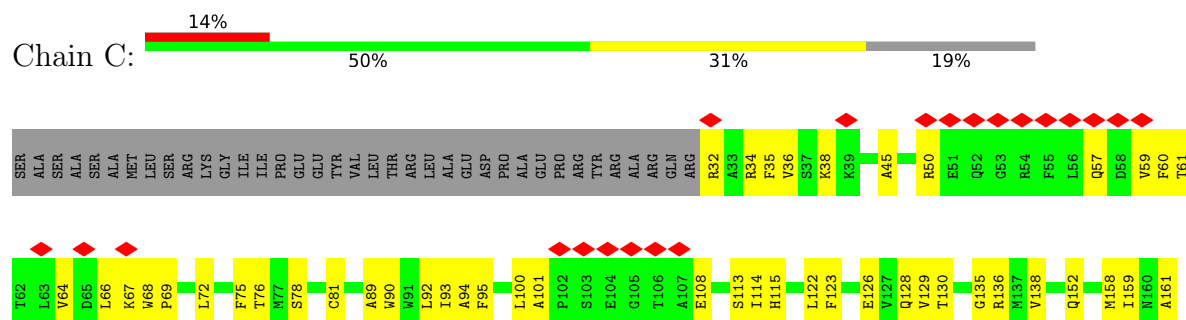
### 3 Residue-property plots

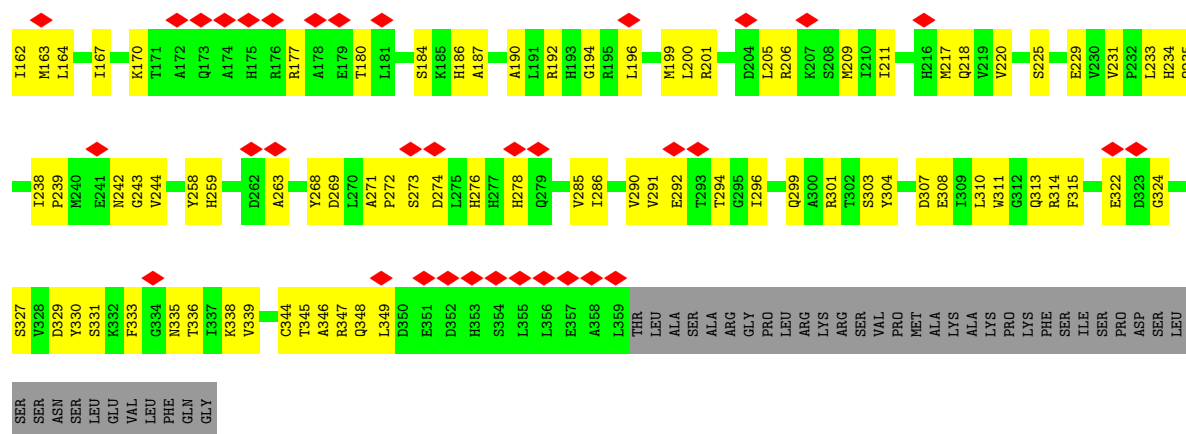
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-sensitive inward rectifier potassium channel 11

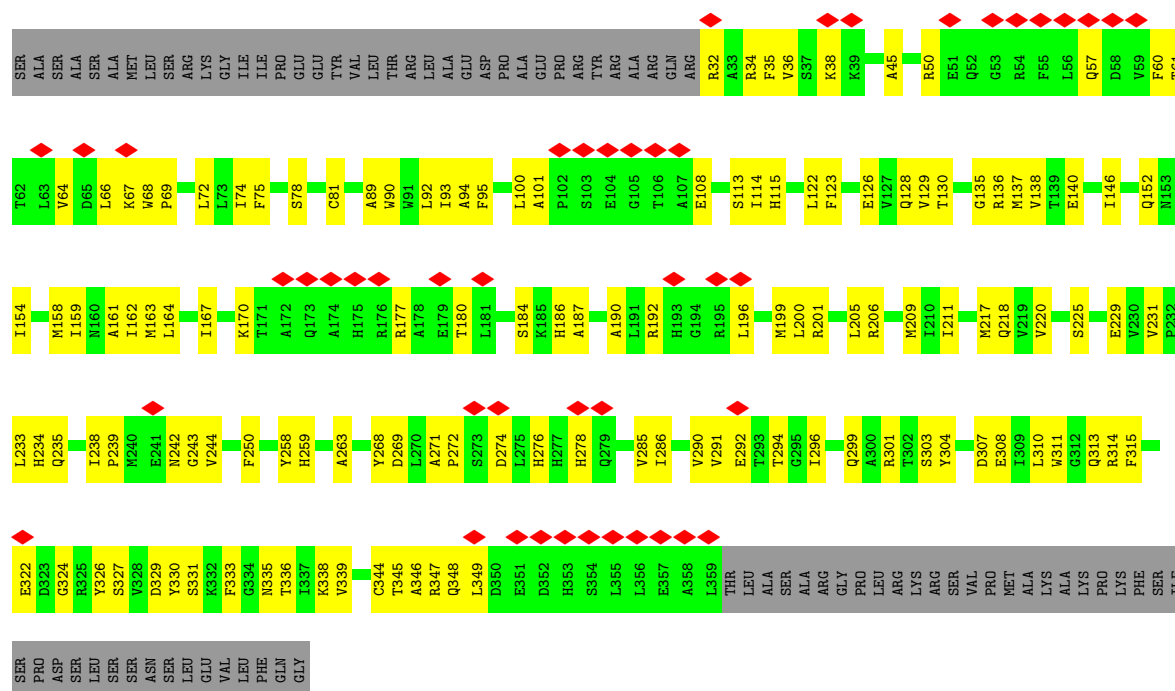


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

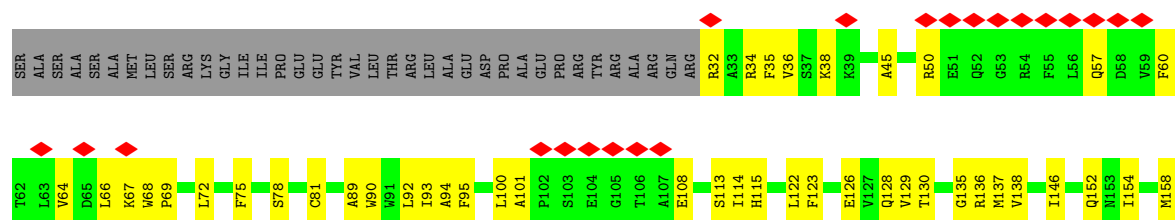




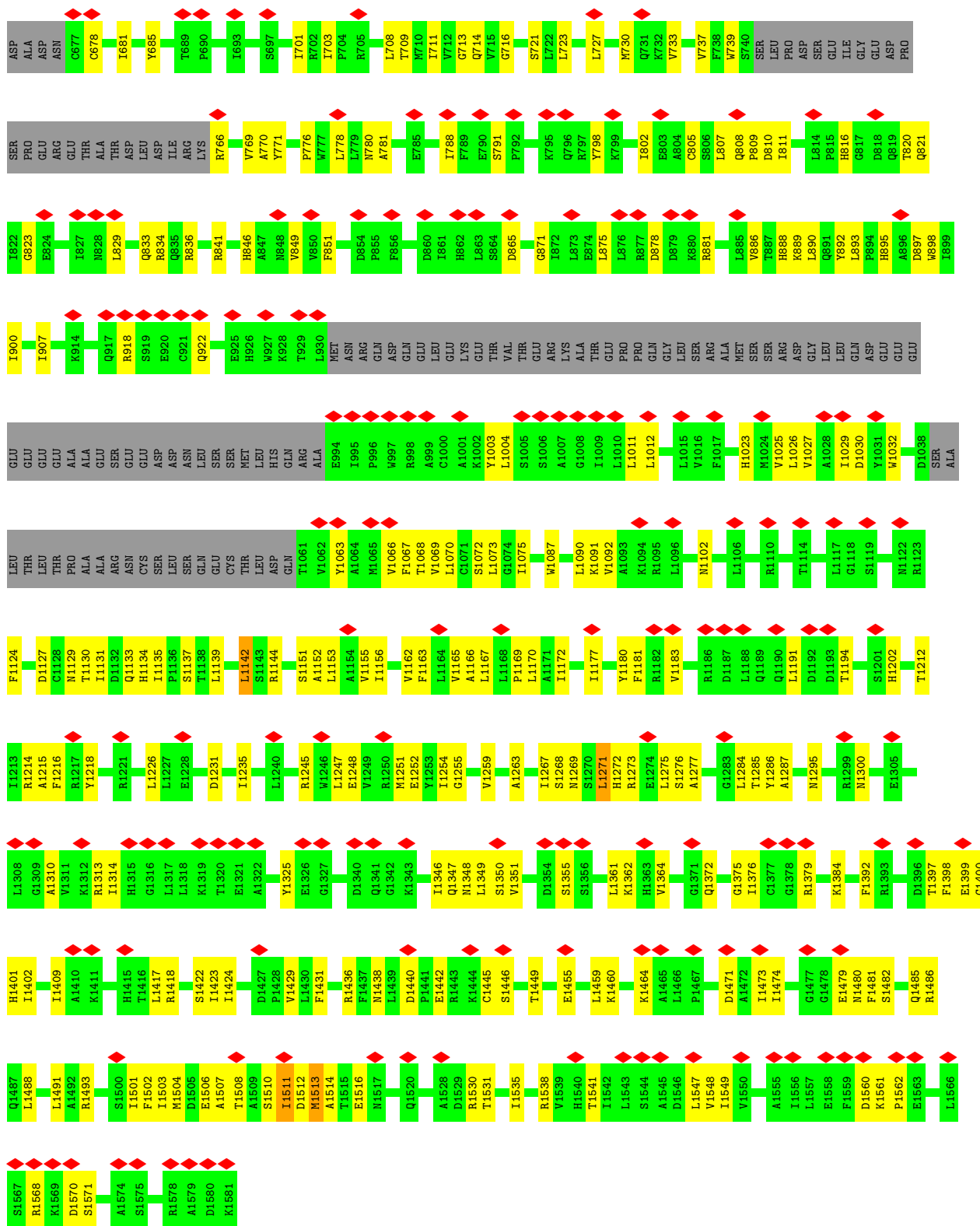
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



- Molecule 1: ATP-sensitive inward rectifier potassium channel 11







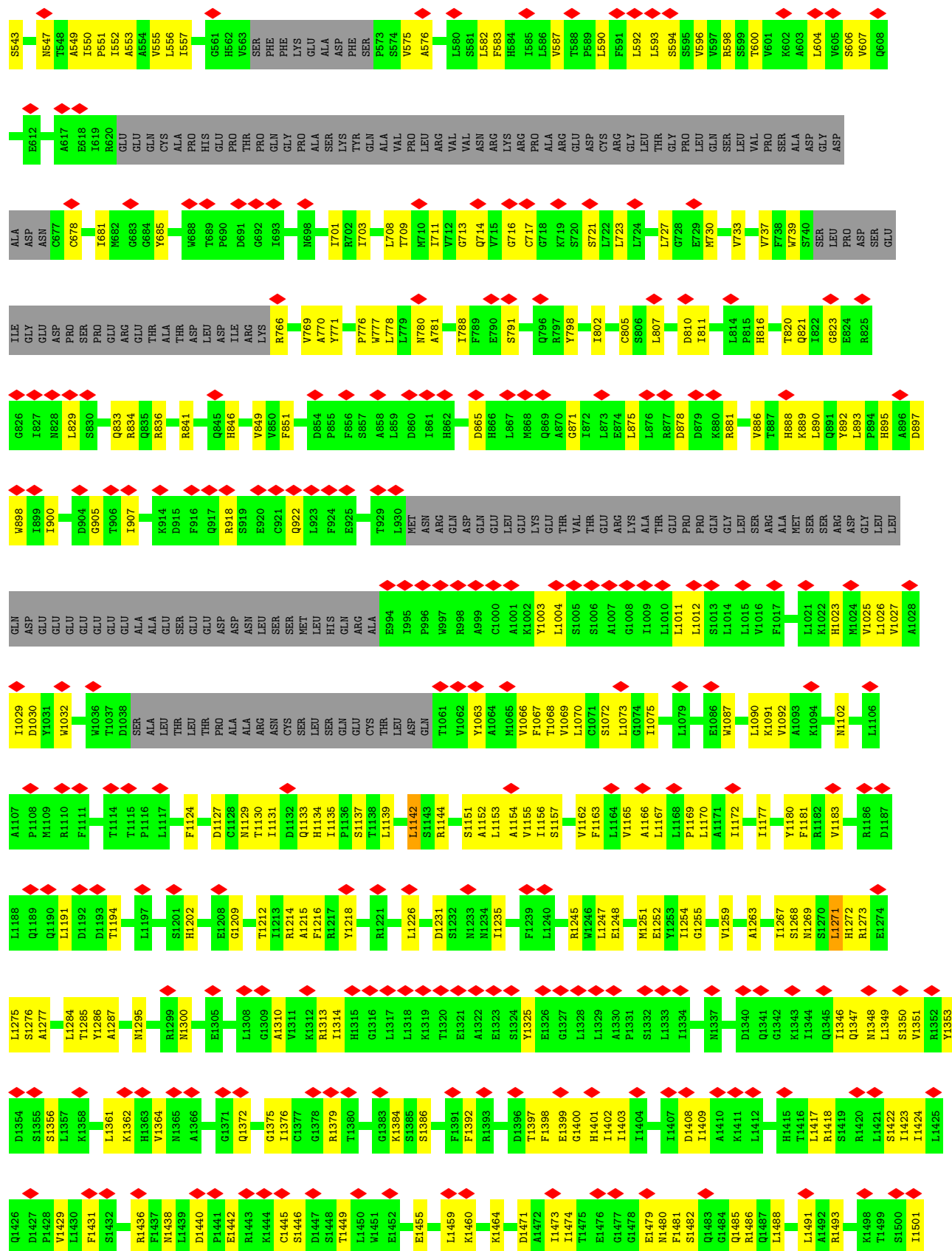


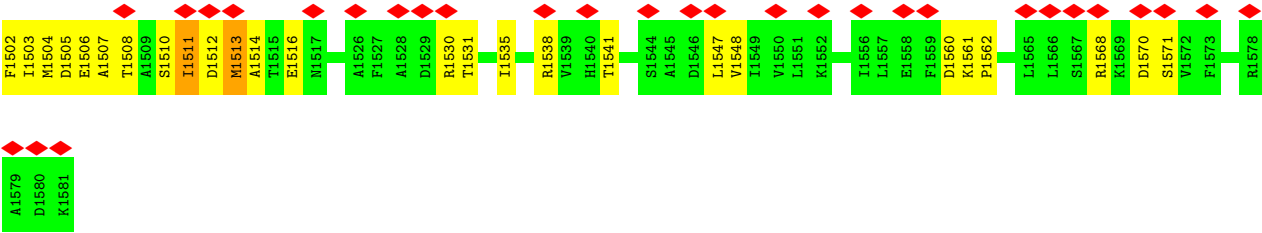












## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C4                               | Depositor |
| Number of particles used             | 47282                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.18                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 2.702                                   | Depositor |
| Minimum map value                    | -1.154                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.020                                   | Depositor |
| Recommended contour level            | 0.117                                   | Depositor |
| Map size (Å)                         | 390.0, 390.0, 390.0                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.3, 1.3, 1.3                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, K, MG, ATP

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.33         | 0/2557  | 0.48        | 0/3482         |
| 1   | B     | 0.32         | 0/2557  | 0.48        | 0/3482         |
| 1   | C     | 0.32         | 0/2557  | 0.48        | 0/3482         |
| 1   | D     | 0.32         | 0/2557  | 0.48        | 0/3482         |
| 2   | E     | 0.28         | 0/9862  | 0.51        | 1/13439 (0.0%) |
| 2   | F     | 0.28         | 0/9862  | 0.51        | 1/13439 (0.0%) |
| 2   | G     | 0.28         | 0/9862  | 0.51        | 1/13439 (0.0%) |
| 2   | H     | 0.28         | 0/9862  | 0.51        | 1/13439 (0.0%) |
| All | All   | 0.29         | 0/49676 | 0.50        | 4/67684 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | F     | 1513 | MET  | N-CA-C | 5.42 | 117.94      | 111.71   |
| 2   | E     | 1513 | MET  | N-CA-C | 5.41 | 117.94      | 111.71   |
| 2   | G     | 1513 | MET  | N-CA-C | 5.37 | 117.89      | 111.71   |
| 2   | H     | 1513 | MET  | N-CA-C | 5.34 | 117.86      | 111.71   |

There are no chirality outliers.

There are no planarity outliers.

### 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   | A     | 2501  | 0        | 2491     | 101     | 0            |
| 1   | B     | 2501  | 0        | 2491     | 105     | 0            |
| 1   | C     | 2501  | 0        | 2491     | 118     | 0            |
| 1   | D     | 2501  | 0        | 2491     | 114     | 0            |
| 2   | E     | 9671  | 0        | 9660     | 281     | 0            |
| 2   | F     | 9671  | 0        | 9660     | 286     | 0            |
| 2   | G     | 9671  | 0        | 9660     | 304     | 0            |
| 2   | H     | 9671  | 0        | 9660     | 294     | 0            |
| 3   | A     | 31    | 0        | 12       | 1       | 0            |
| 3   | B     | 31    | 0        | 12       | 1       | 0            |
| 3   | C     | 31    | 0        | 12       | 1       | 0            |
| 3   | D     | 31    | 0        | 12       | 1       | 0            |
| 3   | E     | 31    | 0        | 12       | 2       | 0            |
| 3   | F     | 31    | 0        | 12       | 2       | 0            |
| 3   | G     | 31    | 0        | 12       | 3       | 0            |
| 3   | H     | 31    | 0        | 12       | 2       | 0            |
| 4   | A     | 3     | 0        | 0        | 0       | 0            |
| 5   | E     | 27    | 0        | 12       | 0       | 0            |
| 5   | F     | 27    | 0        | 12       | 0       | 0            |
| 5   | G     | 27    | 0        | 12       | 0       | 0            |
| 5   | H     | 27    | 0        | 12       | 0       | 0            |
| 6   | E     | 2     | 0        | 0        | 0       | 0            |
| 6   | F     | 2     | 0        | 0        | 0       | 0            |
| 6   | G     | 2     | 0        | 0        | 0       | 0            |
| 6   | H     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 49055 | 0        | 48748    | 1508    | 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 15.

All (1508) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 2:G:888:HIS:ND1 | 2:G:1512:ASP:OD1 | 1.66                     | 1.28              |
| 2:F:888:HIS:ND1 | 2:F:1512:ASP:OD1 | 1.66                     | 1.25              |
| 2:H:888:HIS:ND1 | 2:H:1512:ASP:OD1 | 1.66                     | 1.24              |
| 2:E:888:HIS:ND1 | 2:E:1512:ASP:OD1 | 1.66                     | 1.24              |
| 1:C:276:HIS:CD2 | 2:G:1355:SER:HB2 | 1.89                     | 1.06              |
| 1:C:276:HIS:HD2 | 2:G:1355:SER:HB2 | 1.20                     | 0.98              |
| 1:D:101:ALA:HB2 | 2:H:16:ARG:HB2   | 1.51                     | 0.92              |
| 2:G:888:HIS:CE1 | 2:G:1512:ASP:OD1 | 2.23                     | 0.92              |
| 2:F:888:HIS:CE1 | 2:F:1512:ASP:OD1 | 2.23                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:888:HIS:CE1   | 2:H:1512:ASP:OD1  | 2.23                     | 0.91              |
| 2:E:888:HIS:CE1   | 2:E:1512:ASP:OD1  | 2.23                     | 0.91              |
| 1:D:278:HIS:CG    | 2:H:1356:SER:OG   | 2.24                     | 0.91              |
| 1:A:81:CYS:HB2    | 2:E:41:PHE:HB3    | 1.54                     | 0.89              |
| 2:H:309:ALA:O     | 2:H:369:GLN:NE2   | 2.08                     | 0.87              |
| 1:C:273:SER:OG    | 2:G:1398:PHE:CD2  | 2.27                     | 0.87              |
| 2:F:309:ALA:O     | 2:F:369:GLN:NE2   | 2.08                     | 0.87              |
| 1:C:81:CYS:HB2    | 2:G:41:PHE:HB3    | 1.56                     | 0.86              |
| 1:A:67:LYS:HG2    | 1:A:69:PRO:HD2    | 1.58                     | 0.86              |
| 1:B:67:LYS:HG2    | 1:B:69:PRO:HD2    | 1.58                     | 0.86              |
| 2:E:309:ALA:O     | 2:E:369:GLN:NE2   | 2.08                     | 0.86              |
| 2:G:309:ALA:O     | 2:G:369:GLN:NE2   | 2.08                     | 0.86              |
| 1:C:67:LYS:HG2    | 1:C:69:PRO:HD2    | 1.58                     | 0.85              |
| 1:B:101:ALA:HB2   | 2:F:16:ARG:HB2    | 1.58                     | 0.85              |
| 2:F:723:LEU:HB3   | 2:F:851:PHE:HZ    | 1.41                     | 0.85              |
| 1:D:67:LYS:HG2    | 1:D:69:PRO:HD2    | 1.58                     | 0.84              |
| 1:D:278:HIS:CD2   | 2:H:1356:SER:OG   | 2.30                     | 0.84              |
| 2:G:1510:SER:C    | 2:G:1511:ILE:HD13 | 2.03                     | 0.84              |
| 2:H:496:LEU:HD13  | 2:H:500:ASN:HD21  | 1.43                     | 0.84              |
| 2:H:723:LEU:HB3   | 2:H:851:PHE:HZ    | 1.41                     | 0.83              |
| 2:E:1510:SER:C    | 2:E:1511:ILE:HD13 | 2.03                     | 0.83              |
| 2:F:1510:SER:C    | 2:F:1511:ILE:HD13 | 2.03                     | 0.83              |
| 2:H:1510:SER:C    | 2:H:1511:ILE:HD13 | 2.03                     | 0.83              |
| 2:E:723:LEU:HB3   | 2:E:851:PHE:HZ    | 1.41                     | 0.83              |
| 2:F:496:LEU:HD13  | 2:F:500:ASN:HD21  | 1.43                     | 0.82              |
| 2:E:496:LEU:HD13  | 2:E:500:ASN:HD21  | 1.43                     | 0.82              |
| 2:G:723:LEU:HB3   | 2:G:851:PHE:HZ    | 1.41                     | 0.82              |
| 2:G:496:LEU:HD13  | 2:G:500:ASN:HD21  | 1.43                     | 0.82              |
| 1:D:81:CYS:HB2    | 2:H:41:PHE:HB3    | 1.62                     | 0.80              |
| 2:H:424:ASP:OD1   | 2:H:606:SER:OG    | 2.01                     | 0.79              |
| 2:E:424:ASP:OD1   | 2:E:606:SER:OG    | 2.01                     | 0.78              |
| 2:H:1025:VAL:HG11 | 2:H:1073:LEU:HD22 | 1.66                     | 0.78              |
| 2:H:1508:THR:HA   | 2:H:1511:ILE:HG12 | 1.65                     | 0.78              |
| 2:F:1459:LEU:HD21 | 2:F:1488:LEU:HB3  | 1.66                     | 0.78              |
| 2:H:1459:LEU:HD21 | 2:H:1488:LEU:HB3  | 1.66                     | 0.78              |
| 2:E:1459:LEU:HD21 | 2:E:1488:LEU:HB3  | 1.66                     | 0.78              |
| 2:E:1025:VAL:HG11 | 2:E:1073:LEU:HD22 | 1.66                     | 0.77              |
| 2:G:1459:LEU:HD21 | 2:G:1488:LEU:HB3  | 1.66                     | 0.77              |
| 2:F:424:ASP:OD1   | 2:F:606:SER:OG    | 2.01                     | 0.77              |
| 2:G:424:ASP:OD1   | 2:G:606:SER:OG    | 2.01                     | 0.77              |
| 2:G:1508:THR:HA   | 2:G:1511:ILE:HG12 | 1.66                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:547:ASN:HD22  | 2:F:594:SER:HB2   | 1.50                     | 0.77              |
| 2:G:97:GLY:HA2    | 2:G:1268:SER:HB2  | 1.67                     | 0.77              |
| 1:B:278:HIS:CG    | 2:F:1356:SER:OG   | 2.38                     | 0.77              |
| 2:H:97:GLY:HA2    | 2:H:1268:SER:HB2  | 1.67                     | 0.77              |
| 2:F:97:GLY:HA2    | 2:F:1268:SER:HB2  | 1.67                     | 0.76              |
| 2:F:1508:THR:HA   | 2:F:1511:ILE:HG12 | 1.65                     | 0.76              |
| 1:C:101:ALA:HB2   | 2:G:16:ARG:HB2    | 1.67                     | 0.76              |
| 2:H:547:ASN:HD22  | 2:H:594:SER:HB2   | 1.50                     | 0.76              |
| 2:F:1025:VAL:HG11 | 2:F:1073:LEU:HD22 | 1.66                     | 0.76              |
| 1:B:81:CYS:HB2    | 2:F:41:PHE:HB3    | 1.68                     | 0.76              |
| 2:E:1508:THR:HA   | 2:E:1511:ILE:HG12 | 1.66                     | 0.76              |
| 2:H:714:GLN:C     | 2:H:1512:ASP:OD2  | 2.29                     | 0.76              |
| 2:G:714:GLN:C     | 2:G:1512:ASP:OD2  | 2.29                     | 0.76              |
| 2:G:1025:VAL:HG11 | 2:G:1073:LEU:HD22 | 1.65                     | 0.76              |
| 2:F:714:GLN:C     | 2:F:1512:ASP:OD2  | 2.29                     | 0.76              |
| 2:E:97:GLY:HA2    | 2:E:1268:SER:HB2  | 1.67                     | 0.76              |
| 2:G:547:ASN:HD22  | 2:G:594:SER:HB2   | 1.50                     | 0.76              |
| 2:E:1170:LEU:HD21 | 2:E:1254:ILE:HG23 | 1.68                     | 0.75              |
| 2:H:1216:PHE:HB3  | 2:H:1218:TYR:HD2  | 1.51                     | 0.75              |
| 2:E:714:GLN:C     | 2:E:1512:ASP:OD2  | 2.29                     | 0.75              |
| 2:E:1429:VAL:O    | 2:E:1493:ARG:NH1  | 2.18                     | 0.75              |
| 2:E:1445:CYS:HG   | 2:E:1449:THR:HG1  | 1.30                     | 0.75              |
| 2:G:598:ARG:NH1   | 2:G:1137:SER:OG   | 2.20                     | 0.74              |
| 2:F:1170:LEU:HD21 | 2:F:1254:ILE:HG23 | 1.68                     | 0.74              |
| 2:E:547:ASN:HD22  | 2:E:594:SER:HB2   | 1.50                     | 0.74              |
| 2:H:1429:VAL:O    | 2:H:1493:ARG:NH1  | 2.17                     | 0.74              |
| 2:H:1170:LEU:HD21 | 2:H:1254:ILE:HG23 | 1.68                     | 0.74              |
| 1:A:136:ARG:NH2   | 1:B:138:VAL:O     | 2.18                     | 0.74              |
| 2:E:1216:PHE:HB3  | 2:E:1218:TYR:HD2  | 1.51                     | 0.74              |
| 2:G:1216:PHE:HB3  | 2:G:1218:TYR:HD2  | 1.51                     | 0.74              |
| 2:F:29:ASP:OD2    | 2:F:105:HIS:ND1   | 2.17                     | 0.74              |
| 2:H:598:ARG:NH1   | 2:H:1137:SER:OG   | 2.20                     | 0.74              |
| 2:F:556:LEU:HD11  | 2:F:1068:THR:HG22 | 1.69                     | 0.74              |
| 2:E:598:ARG:NH1   | 2:E:1137:SER:OG   | 2.20                     | 0.74              |
| 2:G:1170:LEU:HD21 | 2:G:1254:ILE:HG23 | 1.68                     | 0.74              |
| 2:G:1429:VAL:O    | 2:G:1493:ARG:NH1  | 2.17                     | 0.74              |
| 2:G:6:CYS:HA      | 2:G:103:HIS:HB2   | 1.70                     | 0.73              |
| 2:F:598:ARG:NH1   | 2:F:1137:SER:OG   | 2.20                     | 0.73              |
| 2:F:1216:PHE:HB3  | 2:F:1218:TYR:HD2  | 1.51                     | 0.73              |
| 2:H:6:CYS:HA      | 2:H:103:HIS:HB2   | 1.70                     | 0.73              |
| 2:G:556:LEU:HD11  | 2:G:1068:THR:HG22 | 1.69                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:711:ILE:HB    | 2:G:886:VAL:HG12  | 1.71                     | 0.73              |
| 2:F:1501:ILE:HG22 | 2:F:1531:THR:HB   | 1.70                     | 0.73              |
| 2:E:6:CYS:HA      | 2:E:103:HIS:HB2   | 1.70                     | 0.73              |
| 2:H:711:ILE:HB    | 2:H:886:VAL:HG12  | 1.71                     | 0.73              |
| 2:H:1501:ILE:HG22 | 2:H:1531:THR:HB   | 1.70                     | 0.73              |
| 2:E:437:ASN:HD22  | 2:E:592:LEU:HD23  | 1.54                     | 0.72              |
| 2:E:1511:ILE:HD13 | 2:E:1511:ILE:N    | 2.04                     | 0.72              |
| 2:F:437:ASN:HD22  | 2:F:592:LEU:HD23  | 1.54                     | 0.72              |
| 2:E:556:LEU:HD11  | 2:E:1068:THR:HG22 | 1.69                     | 0.72              |
| 2:F:6:CYS:HA      | 2:F:103:HIS:HB2   | 1.70                     | 0.72              |
| 2:H:437:ASN:HD22  | 2:H:592:LEU:HD23  | 1.55                     | 0.72              |
| 1:B:34:ARG:HH12   | 1:B:38:LYS:HG2    | 1.54                     | 0.72              |
| 1:D:92:LEU:HD22   | 2:H:34:VAL:HG21   | 1.72                     | 0.72              |
| 2:G:29:ASP:OD2    | 2:G:105:HIS:ND1   | 2.17                     | 0.72              |
| 1:C:34:ARG:HH12   | 1:C:38:LYS:HG2    | 1.54                     | 0.72              |
| 2:E:711:ILE:HB    | 2:E:886:VAL:HG12  | 1.71                     | 0.72              |
| 2:E:1501:ILE:HG22 | 2:E:1531:THR:HB   | 1.70                     | 0.72              |
| 2:H:556:LEU:HD11  | 2:H:1068:THR:HG22 | 1.69                     | 0.72              |
| 2:F:711:ILE:HB    | 2:F:886:VAL:HG12  | 1.71                     | 0.71              |
| 2:H:1511:ILE:HD13 | 2:H:1511:ILE:N    | 2.04                     | 0.71              |
| 1:C:136:ARG:NH2   | 1:D:138:VAL:O     | 2.21                     | 0.71              |
| 2:G:437:ASN:HD22  | 2:G:592:LEU:HD23  | 1.54                     | 0.71              |
| 2:G:1501:ILE:HG22 | 2:G:1531:THR:HB   | 1.70                     | 0.71              |
| 1:C:278:HIS:CG    | 2:G:1356:SER:OG   | 2.44                     | 0.71              |
| 2:E:29:ASP:OD2    | 2:E:105:HIS:ND1   | 2.17                     | 0.71              |
| 2:F:1511:ILE:HD13 | 2:F:1511:ILE:N    | 2.04                     | 0.71              |
| 2:G:1511:ILE:HD13 | 2:G:1511:ILE:N    | 2.04                     | 0.71              |
| 1:B:278:HIS:CD2   | 2:F:1356:SER:OG   | 2.43                     | 0.71              |
| 2:G:739:TRP:HE3   | 2:G:766:ARG:HA    | 1.55                     | 0.71              |
| 2:G:587:VAL:HA    | 2:G:590:LEU:HD12  | 1.72                     | 0.70              |
| 2:H:29:ASP:OD2    | 2:H:105:HIS:ND1   | 2.17                     | 0.70              |
| 2:F:1429:VAL:O    | 2:F:1493:ARG:NH1  | 2.17                     | 0.70              |
| 2:H:1029:ILE:HD12 | 2:H:1070:LEU:HB3  | 1.74                     | 0.70              |
| 2:E:739:TRP:HE3   | 2:E:766:ARG:HA    | 1.55                     | 0.70              |
| 2:G:1029:ILE:HD12 | 2:G:1070:LEU:HB3  | 1.74                     | 0.70              |
| 2:E:1029:ILE:HD12 | 2:E:1070:LEU:HB3  | 1.74                     | 0.70              |
| 2:F:739:TRP:HE3   | 2:F:766:ARG:HA    | 1.55                     | 0.70              |
| 2:F:587:VAL:HA    | 2:F:590:LEU:HD12  | 1.72                     | 0.70              |
| 1:A:34:ARG:HH12   | 1:A:38:LYS:HG2    | 1.54                     | 0.70              |
| 2:E:587:VAL:HA    | 2:E:590:LEU:HD12  | 1.72                     | 0.70              |
| 2:H:739:TRP:HE3   | 2:H:766:ARG:HA    | 1.56                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:66:LEU:O      | 1:B:170:LYS:NZ    | 2.26                     | 0.69              |
| 1:D:34:ARG:HH12   | 1:D:38:LYS:HG2    | 1.54                     | 0.69              |
| 1:D:66:LEU:O      | 1:D:170:LYS:NZ    | 2.26                     | 0.69              |
| 1:A:66:LEU:O      | 1:A:170:LYS:NZ    | 2.26                     | 0.69              |
| 2:E:865:ASP:OD1   | 2:E:892:TYR:OH    | 2.11                     | 0.69              |
| 2:F:1029:ILE:HD12 | 2:F:1070:LEU:HB3  | 1.74                     | 0.69              |
| 1:D:278:HIS:HD1   | 2:H:1355:SER:HG   | 1.40                     | 0.69              |
| 2:H:118:VAL:HG11  | 2:H:1172:ILE:HG21 | 1.75                     | 0.69              |
| 2:H:587:VAL:HA    | 2:H:590:LEU:HD12  | 1.72                     | 0.69              |
| 2:F:118:VAL:HG11  | 2:F:1172:ILE:HG21 | 1.75                     | 0.69              |
| 1:B:192:ARG:NH2   | 1:B:199:MET:SD    | 2.66                     | 0.69              |
| 1:D:192:ARG:NH2   | 1:D:199:MET:SD    | 2.66                     | 0.69              |
| 2:G:118:VAL:HG11  | 2:G:1172:ILE:HG21 | 1.75                     | 0.69              |
| 2:G:865:ASP:OD1   | 2:G:892:TYR:OH    | 2.11                     | 0.68              |
| 1:B:113:SER:OG    | 1:B:135:GLY:O     | 2.12                     | 0.68              |
| 1:C:66:LEU:O      | 1:C:170:LYS:NZ    | 2.26                     | 0.68              |
| 1:C:177:ARG:HH12  | 1:C:206:ARG:HB2   | 1.59                     | 0.68              |
| 1:A:192:ARG:NH2   | 1:A:199:MET:SD    | 2.66                     | 0.68              |
| 1:C:192:ARG:NH2   | 1:C:199:MET:SD    | 2.66                     | 0.68              |
| 1:C:273:SER:OG    | 2:G:1398:PHE:HD2  | 1.75                     | 0.68              |
| 2:E:118:VAL:HG11  | 2:E:1172:ILE:HG21 | 1.75                     | 0.68              |
| 1:B:177:ARG:HH12  | 1:B:206:ARG:HB2   | 1.58                     | 0.68              |
| 2:H:1479:GLU:HA   | 2:H:1486:ARG:HH11 | 1.59                     | 0.68              |
| 2:F:865:ASP:OD1   | 2:F:892:TYR:OH    | 2.11                     | 0.68              |
| 1:A:113:SER:OG    | 1:A:135:GLY:O     | 2.12                     | 0.68              |
| 1:C:278:HIS:CD2   | 2:G:1356:SER:OG   | 2.47                     | 0.68              |
| 2:F:1479:GLU:HA   | 2:F:1486:ARG:HH11 | 1.59                     | 0.68              |
| 1:C:113:SER:OG    | 1:C:135:GLY:O     | 2.12                     | 0.68              |
| 2:F:547:ASN:OD1   | 2:F:590:LEU:HB3   | 1.94                     | 0.68              |
| 1:D:276:HIS:HD2   | 2:H:1355:SER:HB2  | 1.59                     | 0.67              |
| 2:H:322:GLY:O     | 2:H:326:HIS:ND1   | 2.22                     | 0.67              |
| 2:H:1259:VAL:HA   | 2:H:1287:ALA:HB1  | 1.76                     | 0.67              |
| 2:E:1259:VAL:HA   | 2:E:1287:ALA:HB1  | 1.76                     | 0.67              |
| 2:G:547:ASN:OD1   | 2:G:590:LEU:HB3   | 1.94                     | 0.67              |
| 2:E:547:ASN:OD1   | 2:E:590:LEU:HB3   | 1.94                     | 0.67              |
| 1:D:177:ARG:HH12  | 1:D:206:ARG:HB2   | 1.59                     | 0.67              |
| 2:H:865:ASP:OD1   | 2:H:892:TYR:OH    | 2.11                     | 0.67              |
| 2:F:322:GLY:O     | 2:F:326:HIS:ND1   | 2.22                     | 0.67              |
| 1:D:278:HIS:CD2   | 2:H:1356:SER:HG   | 2.12                     | 0.66              |
| 2:G:1259:VAL:HA   | 2:G:1287:ALA:HB1  | 1.76                     | 0.66              |
| 2:F:1259:VAL:HA   | 2:F:1287:ALA:HB1  | 1.76                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1479:GLU:HA   | 2:E:1486:ARG:HH11 | 1.59                     | 0.66              |
| 2:H:547:ASN:OD1   | 2:H:590:LEU:HB3   | 1.94                     | 0.66              |
| 1:A:177:ARG:HH12  | 1:A:206:ARG:HB2   | 1.59                     | 0.66              |
| 1:C:220:VAL:HG22  | 1:C:235:GLN:HG2   | 1.77                     | 0.66              |
| 2:E:370:ARG:HD3   | 2:E:373:LEU:HD12  | 1.77                     | 0.66              |
| 2:G:1479:GLU:HA   | 2:G:1486:ARG:HH11 | 1.59                     | 0.66              |
| 1:D:276:HIS:CD2   | 2:H:1355:SER:HB2  | 2.30                     | 0.66              |
| 1:B:272:PRO:HG3   | 1:B:311:TRP:CE2   | 2.31                     | 0.66              |
| 1:A:272:PRO:HG3   | 1:A:311:TRP:CE2   | 2.31                     | 0.66              |
| 2:H:889:LYS:HB3   | 2:H:1538:ARG:HH22 | 1.61                     | 0.66              |
| 2:G:309:ALA:C     | 2:G:369:GLN:HE22  | 2.04                     | 0.66              |
| 2:F:370:ARG:HD3   | 2:F:373:LEU:HD12  | 1.77                     | 0.66              |
| 1:C:239:PRO:O     | 1:C:259:HIS:ND1   | 2.25                     | 0.66              |
| 1:B:220:VAL:HG22  | 1:B:235:GLN:HG2   | 1.77                     | 0.66              |
| 1:A:220:VAL:HG22  | 1:A:235:GLN:HG2   | 1.77                     | 0.66              |
| 2:G:889:LYS:HB3   | 2:G:1538:ARG:HH22 | 1.61                     | 0.66              |
| 2:E:322:GLY:O     | 2:E:326:HIS:ND1   | 2.22                     | 0.65              |
| 1:C:272:PRO:HG3   | 1:C:311:TRP:CE2   | 2.31                     | 0.65              |
| 1:C:273:SER:HG    | 2:G:1398:PHE:HD2  | 1.39                     | 0.65              |
| 1:D:272:PRO:HG3   | 1:D:311:TRP:CE2   | 2.31                     | 0.65              |
| 1:D:113:SER:OG    | 1:D:135:GLY:O     | 2.12                     | 0.65              |
| 2:E:889:LYS:HB3   | 2:E:1538:ARG:HH22 | 1.61                     | 0.65              |
| 2:F:889:LYS:HB3   | 2:F:1538:ARG:HH22 | 1.61                     | 0.65              |
| 1:D:220:VAL:HG22  | 1:D:235:GLN:HG2   | 1.77                     | 0.65              |
| 2:G:370:ARG:HD3   | 2:G:373:LEU:HD12  | 1.77                     | 0.65              |
| 2:G:1127:ASP:HB3  | 2:G:1314:ILE:HD11 | 1.79                     | 0.65              |
| 2:F:1127:ASP:HB3  | 2:F:1314:ILE:HD11 | 1.79                     | 0.65              |
| 2:H:370:ARG:HD3   | 2:H:373:LEU:HD12  | 1.77                     | 0.65              |
| 1:A:167:ILE:HG21  | 1:B:161:ALA:HB1   | 1.78                     | 0.65              |
| 1:B:239:PRO:O     | 1:B:259:HIS:ND1   | 2.25                     | 0.65              |
| 2:G:322:GLY:O     | 2:G:326:HIS:ND1   | 2.22                     | 0.65              |
| 2:E:1424:ILE:HD12 | 2:E:1504:MET:HG2  | 1.79                     | 0.65              |
| 1:C:278:HIS:ND1   | 2:G:1355:SER:OG   | 2.27                     | 0.64              |
| 2:E:1127:ASP:HB3  | 2:E:1314:ILE:HD11 | 1.79                     | 0.64              |
| 2:G:1011:LEU:HD21 | 2:G:1087:TRP:CE3  | 2.33                     | 0.64              |
| 2:G:314:PHE:CZ    | 2:G:448:GLY:HA2   | 2.33                     | 0.64              |
| 2:H:314:PHE:CZ    | 2:H:448:GLY:HA2   | 2.33                     | 0.64              |
| 2:H:1011:LEU:HD21 | 2:H:1087:TRP:CE3  | 2.33                     | 0.64              |
| 2:F:1011:LEU:HD21 | 2:F:1087:TRP:CE3  | 2.33                     | 0.64              |
| 2:E:1011:LEU:HD21 | 2:E:1087:TRP:CE3  | 2.33                     | 0.64              |
| 2:E:69:PRO:HD2    | 2:E:189:VAL:HG12  | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:69:PRO:HD2    | 2:H:189:VAL:HG12  | 1.80                     | 0.64              |
| 2:E:314:PHE:CZ    | 2:E:448:GLY:HA2   | 2.33                     | 0.63              |
| 2:H:1127:ASP:HB3  | 2:H:1314:ILE:HD11 | 1.79                     | 0.63              |
| 2:F:314:PHE:CZ    | 2:F:448:GLY:HA2   | 2.33                     | 0.63              |
| 1:B:92:LEU:HD22   | 2:F:34:VAL:HG21   | 1.80                     | 0.63              |
| 2:F:1424:ILE:HD12 | 2:F:1504:MET:HG2  | 1.79                     | 0.63              |
| 2:H:309:ALA:C     | 2:H:369:GLN:HE22  | 2.04                     | 0.63              |
| 2:G:1424:ILE:HD12 | 2:G:1504:MET:HG2  | 1.79                     | 0.63              |
| 1:C:273:SER:HB2   | 2:G:1399:GLU:OE2  | 1.99                     | 0.63              |
| 2:H:510:LYS:NZ    | 2:H:1325:TYR:OH   | 2.31                     | 0.63              |
| 2:F:510:LYS:NZ    | 2:F:1325:TYR:OH   | 2.31                     | 0.63              |
| 2:G:510:LYS:NZ    | 2:G:1325:TYR:OH   | 2.31                     | 0.63              |
| 2:G:1409:ILE:HG13 | 2:G:1417:LEU:HD11 | 1.81                     | 0.62              |
| 2:H:1424:ILE:HD12 | 2:H:1504:MET:HG2  | 1.79                     | 0.62              |
| 2:G:69:PRO:HD2    | 2:G:189:VAL:HG12  | 1.80                     | 0.62              |
| 2:F:295:PHE:CZ    | 2:F:383:THR:HB    | 2.34                     | 0.62              |
| 2:F:309:ALA:C     | 2:F:369:GLN:HE22  | 2.04                     | 0.62              |
| 1:A:101:ALA:HB2   | 2:E:16:ARG:HB2    | 1.81                     | 0.62              |
| 2:E:510:LYS:NZ    | 2:E:1325:TYR:OH   | 2.31                     | 0.62              |
| 2:E:723:LEU:HB3   | 2:E:851:PHE:CZ    | 2.31                     | 0.62              |
| 2:H:380:ALA:O     | 2:H:383:THR:OG1   | 2.18                     | 0.62              |
| 2:G:295:PHE:CZ    | 2:G:383:THR:HB    | 2.34                     | 0.62              |
| 2:G:420:LEU:O     | 2:G:424:ASP:HB3   | 2.00                     | 0.62              |
| 2:G:1424:ILE:HD13 | 2:G:1491:LEU:HG   | 1.82                     | 0.62              |
| 1:B:95:PHE:HD1    | 1:B:100:LEU:HD12  | 1.65                     | 0.62              |
| 2:F:69:PRO:HD2    | 2:F:189:VAL:HG12  | 1.80                     | 0.62              |
| 1:D:313:GLN:HG2   | 1:D:338:LYS:HA    | 1.82                     | 0.62              |
| 2:H:829:LEU:HD13  | 2:H:833:GLN:HB2   | 1.82                     | 0.62              |
| 2:E:420:LEU:O     | 2:E:424:ASP:HB3   | 2.00                     | 0.62              |
| 2:E:309:ALA:C     | 2:E:369:GLN:HE22  | 2.04                     | 0.61              |
| 2:H:1424:ILE:HD13 | 2:H:1491:LEU:HG   | 1.82                     | 0.61              |
| 1:A:313:GLN:HG2   | 1:A:338:LYS:HA    | 1.82                     | 0.61              |
| 1:C:167:ILE:HG21  | 1:D:161:ALA:HB1   | 1.81                     | 0.61              |
| 2:E:36:HIS:CE1    | 2:E:113:ALA:HB2   | 2.35                     | 0.61              |
| 2:G:36:HIS:CE1    | 2:G:113:ALA:HB2   | 2.35                     | 0.61              |
| 1:A:239:PRO:O     | 1:A:259:HIS:ND1   | 2.25                     | 0.61              |
| 1:B:313:GLN:HG2   | 1:B:338:LYS:HA    | 1.82                     | 0.61              |
| 2:E:295:PHE:CZ    | 2:E:383:THR:HB    | 2.34                     | 0.61              |
| 2:E:1409:ILE:HG13 | 2:E:1417:LEU:HD11 | 1.81                     | 0.61              |
| 2:H:295:PHE:CZ    | 2:H:383:THR:HB    | 2.34                     | 0.61              |
| 2:F:420:LEU:O     | 2:F:424:ASP:HB3   | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:380:ALA:O     | 2:E:383:THR:OG1   | 2.18                     | 0.61              |
| 2:H:1409:ILE:HG13 | 2:H:1417:LEU:HD11 | 1.81                     | 0.61              |
| 2:F:1409:ILE:HG13 | 2:F:1417:LEU:HD11 | 1.81                     | 0.61              |
| 2:F:74:ARG:HH21   | 2:F:185:VAL:HG12  | 1.66                     | 0.61              |
| 1:C:95:PHE:HD1    | 1:C:100:LEU:HD12  | 1.65                     | 0.61              |
| 2:H:420:LEU:O     | 2:H:424:ASP:HB3   | 2.00                     | 0.61              |
| 2:H:723:LEU:HB3   | 2:H:851:PHE:CZ    | 2.31                     | 0.61              |
| 2:E:74:ARG:HH21   | 2:E:185:VAL:HG12  | 1.66                     | 0.61              |
| 2:E:829:LEU:HD13  | 2:E:833:GLN:HB2   | 1.82                     | 0.61              |
| 2:E:1560:ASP:OD1  | 2:E:1561:LYS:N    | 2.32                     | 0.61              |
| 2:G:829:LEU:HD13  | 2:G:833:GLN:HB2   | 1.82                     | 0.61              |
| 2:F:1482:SER:OG   | 3:F:2004:ATP:O3A  | 2.19                     | 0.61              |
| 2:E:78:THR:HG21   | 2:E:121:VAL:HG21  | 1.82                     | 0.61              |
| 2:F:829:LEU:HD13  | 2:F:833:GLN:HB2   | 1.82                     | 0.61              |
| 1:C:61:THR:HA     | 1:C:64:VAL:HG12   | 1.82                     | 0.60              |
| 1:C:92:LEU:HD22   | 2:G:34:VAL:HG21   | 1.83                     | 0.60              |
| 1:C:158:MET:HE2   | 1:B:72:LEU:HD23   | 1.82                     | 0.60              |
| 1:D:95:PHE:HD1    | 1:D:100:LEU:HD12  | 1.65                     | 0.60              |
| 2:H:36:HIS:CE1    | 2:H:113:ALA:HB2   | 2.35                     | 0.60              |
| 2:G:74:ARG:HH21   | 2:G:185:VAL:HG12  | 1.66                     | 0.60              |
| 2:F:36:HIS:CE1    | 2:F:113:ALA:HB2   | 2.35                     | 0.60              |
| 2:F:380:ALA:O     | 2:F:383:THR:OG1   | 2.18                     | 0.60              |
| 2:E:1482:SER:OG   | 3:E:2004:ATP:O3A  | 2.19                     | 0.60              |
| 2:G:412:MET:HA    | 2:G:416:GLN:HE21  | 1.66                     | 0.60              |
| 1:B:61:THR:HA     | 1:B:64:VAL:HG12   | 1.82                     | 0.60              |
| 2:G:1473:ILE:O    | 2:G:1480:ASN:ND2  | 2.34                     | 0.60              |
| 2:F:810:ASP:OD2   | 2:F:836:ARG:NH2   | 2.35                     | 0.60              |
| 1:A:95:PHE:HD1    | 1:A:100:LEU:HD12  | 1.65                     | 0.60              |
| 1:C:313:GLN:HG2   | 1:C:338:LYS:HA    | 1.82                     | 0.60              |
| 1:D:239:PRO:O     | 1:D:259:HIS:ND1   | 2.25                     | 0.60              |
| 2:F:78:THR:HG21   | 2:F:121:VAL:HG21  | 1.82                     | 0.60              |
| 2:F:412:MET:HA    | 2:F:416:GLN:HE21  | 1.66                     | 0.60              |
| 2:F:1424:ILE:HD13 | 2:F:1491:LEU:HG   | 1.82                     | 0.60              |
| 1:A:61:THR:HA     | 1:A:64:VAL:HG12   | 1.82                     | 0.60              |
| 1:D:314:ARG:HE    | 1:D:339:VAL:HG21  | 1.66                     | 0.60              |
| 2:E:8:SER:H       | 2:E:12:SER:CB     | 2.14                     | 0.60              |
| 2:E:1424:ILE:HD13 | 2:E:1491:LEU:HG   | 1.82                     | 0.60              |
| 2:H:412:MET:HA    | 2:H:416:GLN:HE21  | 1.66                     | 0.60              |
| 2:H:1473:ILE:O    | 2:H:1480:ASN:ND2  | 2.34                     | 0.60              |
| 2:G:78:THR:HG21   | 2:G:121:VAL:HG21  | 1.82                     | 0.60              |
| 2:F:1263:ALA:O    | 2:F:1267:ILE:HG12 | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:78:THR:HG21   | 2:H:121:VAL:HG21  | 1.82                     | 0.60              |
| 2:H:810:ASP:OD2   | 2:H:836:ARG:NH2   | 2.35                     | 0.60              |
| 2:G:8:SER:H       | 2:G:12:SER:CB     | 2.14                     | 0.60              |
| 2:F:452:LEU:HB3   | 2:F:461:LEU:HD22  | 1.84                     | 0.60              |
| 2:F:770:ALA:HA    | 2:F:1216:PHE:HE1  | 1.67                     | 0.60              |
| 1:D:61:THR:HA     | 1:D:64:VAL:HG12   | 1.82                     | 0.60              |
| 2:H:74:ARG:HH21   | 2:H:185:VAL:HG12  | 1.66                     | 0.60              |
| 2:G:1350:SER:HB2  | 2:G:1399:GLU:HB2  | 1.84                     | 0.60              |
| 2:F:8:SER:H       | 2:F:12:SER:CB     | 2.14                     | 0.60              |
| 1:C:314:ARG:HE    | 1:C:339:VAL:HG21  | 1.66                     | 0.60              |
| 2:E:1263:ALA:O    | 2:E:1267:ILE:HG12 | 2.02                     | 0.60              |
| 2:E:1350:SER:HB2  | 2:E:1399:GLU:HB2  | 1.84                     | 0.60              |
| 2:G:288:TRP:HE1   | 2:G:607:VAL:HG21  | 1.67                     | 0.60              |
| 2:G:810:ASP:OD2   | 2:G:836:ARG:NH2   | 2.35                     | 0.60              |
| 1:C:273:SER:OG    | 2:G:1398:PHE:CE2  | 2.51                     | 0.60              |
| 1:B:218:GLN:HE21  | 1:B:235:GLN:HB3   | 1.67                     | 0.60              |
| 2:H:770:ALA:HA    | 2:H:1216:PHE:HE1  | 1.67                     | 0.60              |
| 2:H:1482:SER:OG   | 3:H:2004:ATP:O3A  | 2.19                     | 0.60              |
| 2:F:1473:ILE:O    | 2:F:1480:ASN:ND2  | 2.34                     | 0.60              |
| 1:C:218:GLN:HE21  | 1:C:235:GLN:HB3   | 1.67                     | 0.60              |
| 3:C:501:ATP:N1    | 1:D:50:ARG:N      | 2.47                     | 0.60              |
| 2:G:452:LEU:HB3   | 2:G:461:LEU:HD22  | 1.84                     | 0.60              |
| 1:B:238:ILE:HD11  | 1:B:259:HIS:CD2   | 2.37                     | 0.59              |
| 2:G:778:LEU:HA    | 2:G:841:ARG:HH12  | 1.67                     | 0.59              |
| 1:D:238:ILE:HD11  | 1:D:259:HIS:CD2   | 2.37                     | 0.59              |
| 2:H:1263:ALA:O    | 2:H:1267:ILE:HG12 | 2.02                     | 0.59              |
| 2:H:1350:SER:HB2  | 2:H:1399:GLU:HB2  | 1.84                     | 0.59              |
| 2:E:288:TRP:HE1   | 2:E:607:VAL:HG21  | 1.67                     | 0.59              |
| 2:E:412:MET:HA    | 2:E:416:GLN:HE21  | 1.66                     | 0.59              |
| 2:E:452:LEU:HB3   | 2:E:461:LEU:HD22  | 1.84                     | 0.59              |
| 2:E:1473:ILE:O    | 2:E:1480:ASN:ND2  | 2.34                     | 0.59              |
| 2:H:288:TRP:HE1   | 2:H:607:VAL:HG21  | 1.67                     | 0.59              |
| 2:H:1027:VAL:HG21 | 2:H:1151:SER:HB2  | 1.84                     | 0.59              |
| 2:F:114:PHE:CE2   | 2:F:1169:PRO:HB3  | 2.37                     | 0.59              |
| 2:F:778:LEU:HA    | 2:F:841:ARG:HH12  | 1.67                     | 0.59              |
| 1:A:95:PHE:HE1    | 2:E:16:ARG:HG2    | 1.67                     | 0.59              |
| 2:H:452:LEU:HB3   | 2:H:461:LEU:HD22  | 1.84                     | 0.59              |
| 2:G:1263:ALA:O    | 2:G:1267:ILE:HG12 | 2.02                     | 0.59              |
| 2:G:1482:SER:OG   | 3:G:2004:ATP:O3A  | 2.19                     | 0.59              |
| 2:F:319:CYS:SG    | 2:F:362:LEU:HB2   | 2.42                     | 0.59              |
| 2:F:1027:VAL:HG21 | 2:F:1151:SER:HB2  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:218:GLN:HE21  | 1:A:235:GLN:HB3   | 1.67                     | 0.59              |
| 1:D:218:GLN:HE21  | 1:D:235:GLN:HB3   | 1.67                     | 0.59              |
| 2:E:810:ASP:OD2   | 2:E:836:ARG:NH2   | 2.35                     | 0.59              |
| 2:E:1216:PHE:HB3  | 2:E:1218:TYR:CD2  | 2.37                     | 0.59              |
| 2:H:8:SER:H       | 2:H:12:SER:CB     | 2.14                     | 0.59              |
| 2:H:1216:PHE:HB3  | 2:H:1218:TYR:CD2  | 2.37                     | 0.59              |
| 2:G:114:PHE:CE2   | 2:G:1169:PRO:HB3  | 2.37                     | 0.59              |
| 2:G:319:CYS:SG    | 2:G:362:LEU:HB2   | 2.42                     | 0.59              |
| 2:G:1560:ASP:OD1  | 2:G:1561:LYS:N    | 2.32                     | 0.59              |
| 1:A:314:ARG:HE    | 1:A:339:VAL:HG21  | 1.66                     | 0.59              |
| 1:C:238:ILE:HD11  | 1:C:259:HIS:CD2   | 2.37                     | 0.59              |
| 2:E:1027:VAL:HG21 | 2:E:1151:SER:HB2  | 1.85                     | 0.59              |
| 2:H:114:PHE:CE2   | 2:H:1169:PRO:HB3  | 2.38                     | 0.59              |
| 1:B:314:ARG:HE    | 1:B:339:VAL:HG21  | 1.66                     | 0.59              |
| 1:D:217:MET:HG2   | 1:D:285:VAL:HG22  | 1.84                     | 0.59              |
| 2:E:770:ALA:HA    | 2:E:1216:PHE:HE1  | 1.67                     | 0.59              |
| 2:G:496:LEU:HD13  | 2:G:500:ASN:ND2   | 2.16                     | 0.59              |
| 2:G:1027:VAL:HG21 | 2:G:1151:SER:HB2  | 1.84                     | 0.59              |
| 2:F:496:LEU:HD13  | 2:F:500:ASN:ND2   | 2.16                     | 0.59              |
| 2:F:1350:SER:HB2  | 2:F:1399:GLU:HB2  | 1.84                     | 0.59              |
| 1:B:217:MET:HG2   | 1:B:285:VAL:HG22  | 1.84                     | 0.59              |
| 2:E:320:ILE:HG12  | 2:E:1284:LEU:HD13 | 1.85                     | 0.59              |
| 2:E:778:LEU:HA    | 2:E:841:ARG:HH12  | 1.67                     | 0.59              |
| 2:H:1560:ASP:OD1  | 2:H:1561:LYS:N    | 2.33                     | 0.59              |
| 2:G:320:ILE:HG12  | 2:G:1284:LEU:HD13 | 1.85                     | 0.59              |
| 1:A:238:ILE:HD11  | 1:A:259:HIS:CD2   | 2.37                     | 0.59              |
| 2:E:319:CYS:SG    | 2:E:362:LEU:HB2   | 2.42                     | 0.59              |
| 1:C:217:MET:HG2   | 1:C:285:VAL:HG22  | 1.84                     | 0.58              |
| 2:F:918:ARG:NH2   | 2:F:922:GLN:OE1   | 2.36                     | 0.58              |
| 2:H:319:CYS:SG    | 2:H:362:LEU:HB2   | 2.42                     | 0.58              |
| 2:H:1516:GLU:OE2  | 2:H:1541:THR:OG1  | 2.21                     | 0.58              |
| 2:G:770:ALA:HA    | 2:G:1216:PHE:HE1  | 1.67                     | 0.58              |
| 2:F:320:ILE:HG12  | 2:F:1284:LEU:HD13 | 1.85                     | 0.58              |
| 1:A:50:ARG:N      | 3:D:501:ATP:N1    | 2.45                     | 0.58              |
| 1:B:276:HIS:NE2   | 1:B:278:HIS:O     | 2.37                     | 0.58              |
| 2:E:114:PHE:CE2   | 2:E:1169:PRO:HB3  | 2.37                     | 0.58              |
| 2:E:477:VAL:HG11  | 2:E:543:SER:HB2   | 1.85                     | 0.58              |
| 2:G:380:ALA:O     | 2:G:383:THR:OG1   | 2.18                     | 0.58              |
| 2:F:288:TRP:HE1   | 2:F:607:VAL:HG21  | 1.67                     | 0.58              |
| 2:H:320:ILE:HG12  | 2:H:1284:LEU:HD13 | 1.85                     | 0.58              |
| 2:F:477:VAL:HG11  | 2:F:543:SER:HB2   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:273:SER:OG    | 2:H:1398:PHE:CE2 | 2.56                     | 0.58              |
| 1:A:276:HIS:NE2   | 1:A:278:HIS:O    | 2.37                     | 0.58              |
| 1:C:276:HIS:NE2   | 1:C:278:HIS:O    | 2.37                     | 0.58              |
| 2:F:723:LEU:HB3   | 2:F:851:PHE:CZ   | 2.31                     | 0.58              |
| 2:G:477:VAL:HG11  | 2:G:543:SER:HB2  | 1.85                     | 0.58              |
| 1:A:239:PRO:HB3   | 1:D:244:VAL:HG22 | 1.86                     | 0.58              |
| 2:E:918:ARG:NH2   | 2:E:922:GLN:OE1  | 2.36                     | 0.58              |
| 2:H:318:LEU:HD21  | 2:H:451:LEU:HD21 | 1.86                     | 0.58              |
| 2:H:477:VAL:HG11  | 2:H:543:SER:HB2  | 1.85                     | 0.58              |
| 2:H:555:VAL:HG12  | 2:H:583:PHE:HD2  | 1.69                     | 0.58              |
| 2:H:778:LEU:HA    | 2:H:841:ARG:HH12 | 1.67                     | 0.58              |
| 2:G:918:ARG:NH2   | 2:G:922:GLN:OE1  | 2.36                     | 0.58              |
| 1:A:217:MET:HG2   | 1:A:285:VAL:HG22 | 1.85                     | 0.57              |
| 1:C:75:PHE:O      | 1:C:78:SER:OG    | 2.19                     | 0.57              |
| 1:D:276:HIS:NE2   | 1:D:278:HIS:O    | 2.37                     | 0.57              |
| 2:H:455:ILE:HG23  | 2:H:456:LEU:HG   | 1.86                     | 0.57              |
| 2:H:1436:ARG:NH2  | 2:H:1471:ASP:OD1 | 2.37                     | 0.57              |
| 2:G:318:LEU:HD21  | 2:G:451:LEU:HD21 | 1.86                     | 0.57              |
| 2:G:1436:ARG:NH2  | 2:G:1471:ASP:OD1 | 2.37                     | 0.57              |
| 2:F:776:PRO:O     | 2:F:834:ARG:NH2  | 2.37                     | 0.57              |
| 2:F:1516:GLU:OE2  | 2:F:1541:THR:OG1 | 2.21                     | 0.57              |
| 2:H:496:LEU:HD13  | 2:H:500:ASN:ND2  | 2.16                     | 0.57              |
| 2:H:918:ARG:NH2   | 2:H:922:GLN:OE1  | 2.36                     | 0.57              |
| 2:F:318:LEU:HD21  | 2:F:451:LEU:HD21 | 1.87                     | 0.57              |
| 2:F:1351:VAL:HG22 | 2:F:1361:LEU:HB3 | 1.87                     | 0.57              |
| 2:H:1153:LEU:HD11 | 2:H:1167:LEU:HG  | 1.87                     | 0.57              |
| 2:F:1153:LEU:HD11 | 2:F:1167:LEU:HG  | 1.87                     | 0.57              |
| 1:A:158:MET:HE2   | 1:D:72:LEU:HD23  | 1.85                     | 0.57              |
| 2:G:723:LEU:HB3   | 2:G:851:PHE:CZ   | 2.31                     | 0.57              |
| 2:F:456:LEU:HD22  | 2:F:575:VAL:HA   | 1.87                     | 0.57              |
| 2:E:1351:VAL:HG22 | 2:E:1361:LEU:HB3 | 1.87                     | 0.57              |
| 2:E:318:LEU:HD21  | 2:E:451:LEU:HD21 | 1.86                     | 0.57              |
| 2:E:776:PRO:O     | 2:E:834:ARG:NH2  | 2.37                     | 0.57              |
| 2:G:1153:LEU:HD11 | 2:G:1167:LEU:HG  | 1.87                     | 0.57              |
| 2:F:1436:ARG:NH2  | 2:F:1471:ASP:OD1 | 2.37                     | 0.57              |
| 1:C:239:PRO:HB3   | 1:B:244:VAL:HG22 | 1.85                     | 0.57              |
| 1:C:278:HIS:HD1   | 2:G:1355:SER:HG  | 1.52                     | 0.57              |
| 2:E:455:ILE:HG23  | 2:E:456:LEU:HG   | 1.86                     | 0.57              |
| 2:E:1436:ARG:NH2  | 2:E:1471:ASP:OD1 | 2.37                     | 0.57              |
| 2:H:776:PRO:O     | 2:H:834:ARG:NH2  | 2.38                     | 0.57              |
| 2:G:455:ILE:HG23  | 2:G:456:LEU:HG   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1516:GLU:OE2  | 2:G:1541:THR:OG1  | 2.21                     | 0.57              |
| 2:G:555:VAL:HG12  | 2:G:583:PHE:HD2   | 1.69                     | 0.56              |
| 2:E:117:ALA:O     | 2:E:120:SER:OG    | 2.17                     | 0.56              |
| 2:G:1351:VAL:HG22 | 2:G:1361:LEU:HB3  | 1.87                     | 0.56              |
| 1:C:122:LEU:HD21  | 1:D:146:ILE:HG12  | 1.87                     | 0.56              |
| 2:E:456:LEU:HD22  | 2:E:575:VAL:HA    | 1.87                     | 0.56              |
| 2:E:555:VAL:HG12  | 2:E:583:PHE:HD2   | 1.69                     | 0.56              |
| 2:E:1153:LEU:HD11 | 2:E:1167:LEU:HG   | 1.87                     | 0.56              |
| 2:G:776:PRO:O     | 2:G:834:ARG:NH2   | 2.37                     | 0.56              |
| 1:A:75:PHE:O      | 1:A:78:SER:OG     | 2.19                     | 0.56              |
| 2:F:455:ILE:HG23  | 2:F:456:LEU:HG    | 1.85                     | 0.56              |
| 2:F:1560:ASP:OD1  | 2:F:1561:LYS:N    | 2.33                     | 0.56              |
| 2:E:496:LEU:HD13  | 2:E:500:ASN:ND2   | 2.16                     | 0.56              |
| 2:E:711:ILE:HG13  | 2:E:900:ILE:HB    | 1.87                     | 0.56              |
| 1:C:211:ILE:HB    | 1:C:290:VAL:HB    | 1.87                     | 0.56              |
| 1:B:211:ILE:HB    | 1:B:290:VAL:HB    | 1.88                     | 0.56              |
| 2:G:498:GLN:HE22  | 2:G:521:ARG:NH1   | 2.04                     | 0.56              |
| 2:H:498:GLN:HE22  | 2:H:521:ARG:NH1   | 2.04                     | 0.56              |
| 2:F:498:GLN:HE22  | 2:F:521:ARG:NH1   | 2.04                     | 0.56              |
| 2:H:1191:LEU:HA   | 2:H:1194:THR:HG22 | 1.88                     | 0.56              |
| 2:G:1191:LEU:HA   | 2:G:1194:THR:HG22 | 1.88                     | 0.56              |
| 2:F:555:VAL:HG12  | 2:F:583:PHE:HD2   | 1.69                     | 0.56              |
| 2:G:711:ILE:HG13  | 2:G:900:ILE:HB    | 1.87                     | 0.55              |
| 2:H:1351:VAL:HG22 | 2:H:1361:LEU:HB3  | 1.87                     | 0.55              |
| 2:F:1191:LEU:HA   | 2:F:1194:THR:HG22 | 1.88                     | 0.55              |
| 2:E:498:GLN:HE22  | 2:E:521:ARG:NH1   | 2.04                     | 0.55              |
| 1:A:161:ALA:HB1   | 1:D:167:ILE:HG21  | 1.87                     | 0.55              |
| 2:E:1191:LEU:HA   | 2:E:1194:THR:HG22 | 1.88                     | 0.55              |
| 2:H:117:ALA:O     | 2:H:120:SER:OG    | 2.17                     | 0.55              |
| 2:H:711:ILE:HG13  | 2:H:900:ILE:HB    | 1.87                     | 0.55              |
| 2:H:456:LEU:HD22  | 2:H:575:VAL:HA    | 1.87                     | 0.55              |
| 2:F:14:ALA:HA     | 2:F:17:VAL:HG13   | 1.89                     | 0.55              |
| 2:F:381:ILE:HG13  | 2:F:433:PHE:CE1   | 2.42                     | 0.55              |
| 2:F:455:ILE:O     | 2:F:457:GLY:N     | 2.40                     | 0.55              |
| 2:F:711:ILE:HG13  | 2:F:900:ILE:HB    | 1.87                     | 0.55              |
| 1:D:269:ASP:OD1   | 1:D:347:ARG:NE    | 2.33                     | 0.55              |
| 1:A:211:ILE:HB    | 1:A:290:VAL:HB    | 1.88                     | 0.55              |
| 1:D:75:PHE:O      | 1:D:78:SER:OG     | 2.19                     | 0.55              |
| 2:E:295:PHE:HZ    | 2:E:383:THR:HB    | 1.72                     | 0.55              |
| 2:E:1506:GLU:H    | 2:E:1535:ILE:HB   | 1.72                     | 0.55              |
| 2:G:14:ALA:HA     | 2:G:17:VAL:HG13   | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:138:VAL:O     | 1:D:136:ARG:NH2   | 2.32                     | 0.54              |
| 2:E:388:ARG:NH1   | 2:E:429:MET:SD    | 2.80                     | 0.54              |
| 2:E:455:ILE:O     | 2:E:457:GLY:N     | 2.40                     | 0.54              |
| 2:H:388:ARG:NH1   | 2:H:429:MET:SD    | 2.80                     | 0.54              |
| 2:G:388:ARG:NH1   | 2:G:429:MET:SD    | 2.81                     | 0.54              |
| 2:G:455:ILE:O     | 2:G:457:GLY:N     | 2.40                     | 0.54              |
| 2:E:14:ALA:HA     | 2:E:17:VAL:HG13   | 1.89                     | 0.54              |
| 2:G:456:LEU:HD22  | 2:G:575:VAL:HA    | 1.87                     | 0.54              |
| 2:F:404:THR:OG1   | 2:F:1214:ARG:NH2  | 2.41                     | 0.54              |
| 2:F:1506:GLU:H    | 2:F:1535:ILE:HB   | 1.72                     | 0.54              |
| 2:H:455:ILE:O     | 2:H:457:GLY:N     | 2.40                     | 0.54              |
| 2:F:388:ARG:NH1   | 2:F:429:MET:SD    | 2.80                     | 0.54              |
| 2:E:708:LEU:O     | 2:E:897:ASP:N     | 2.40                     | 0.54              |
| 2:H:14:ALA:HA     | 2:H:17:VAL:HG13   | 1.89                     | 0.54              |
| 2:H:1506:GLU:H    | 2:H:1535:ILE:HB   | 1.72                     | 0.54              |
| 2:G:1506:GLU:H    | 2:G:1535:ILE:HB   | 1.72                     | 0.54              |
| 2:E:381:ILE:HG13  | 2:E:433:PHE:CE1   | 2.42                     | 0.54              |
| 2:H:33:VAL:HG22   | 2:H:109:PRO:HB3   | 1.89                     | 0.54              |
| 2:G:381:ILE:HG13  | 2:G:433:PHE:CE1   | 2.42                     | 0.54              |
| 1:C:129:VAL:O     | 1:C:130:THR:OG1   | 2.23                     | 0.54              |
| 1:D:211:ILE:HB    | 1:D:290:VAL:HB    | 1.88                     | 0.54              |
| 2:E:102:HIS:HD2   | 2:E:1273:ARG:HH11 | 1.56                     | 0.54              |
| 2:E:1516:GLU:OE2  | 2:E:1541:THR:OG1  | 2.21                     | 0.54              |
| 2:H:295:PHE:HZ    | 2:H:383:THR:HB    | 1.73                     | 0.54              |
| 2:H:1177:ILE:HD11 | 2:H:1251:MET:SD   | 2.48                     | 0.54              |
| 2:G:480:LYS:HG3   | 2:G:539:TYR:CE2   | 2.43                     | 0.54              |
| 2:F:117:ALA:O     | 2:F:120:SER:OG    | 2.17                     | 0.54              |
| 2:H:102:HIS:HD2   | 2:H:1273:ARG:HH11 | 1.56                     | 0.54              |
| 2:G:404:THR:OG1   | 2:G:1214:ARG:NH2  | 2.41                     | 0.54              |
| 2:F:708:LEU:O     | 2:F:897:ASP:N     | 2.41                     | 0.54              |
| 1:A:129:VAL:O     | 1:A:130:THR:OG1   | 2.23                     | 0.54              |
| 2:H:381:ILE:HG13  | 2:H:433:PHE:CE1   | 2.42                     | 0.54              |
| 2:F:1216:PHE:HB3  | 2:F:1218:TYR:CD2  | 2.37                     | 0.54              |
| 2:G:6:CYS:H       | 2:G:16:ARG:NH1    | 2.06                     | 0.54              |
| 2:G:708:LEU:O     | 2:G:897:ASP:N     | 2.41                     | 0.54              |
| 2:G:1177:ILE:HD11 | 2:G:1251:MET:SD   | 2.48                     | 0.54              |
| 2:F:1177:ILE:HD11 | 2:F:1251:MET:SD   | 2.48                     | 0.54              |
| 2:E:33:VAL:HG22   | 2:E:109:PRO:HB3   | 1.89                     | 0.53              |
| 2:E:1177:ILE:HD11 | 2:E:1251:MET:SD   | 2.48                     | 0.53              |
| 2:H:404:THR:OG1   | 2:H:1214:ARG:NH2  | 2.40                     | 0.53              |
| 2:G:102:HIS:HD2   | 2:G:1273:ARG:HH11 | 1.56                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:495:ARG:NH1  | 2:G:1124:PHE:O    | 2.38                     | 0.53              |
| 2:G:727:LEU:HD21 | 2:G:1215:ALA:HB2  | 1.90                     | 0.53              |
| 2:E:404:THR:OG1  | 2:E:1214:ARG:NH2  | 2.41                     | 0.53              |
| 2:E:575:VAL:HG23 | 2:E:576:ALA:H     | 1.74                     | 0.53              |
| 2:E:1066:VAL:HA  | 2:E:1069:VAL:HG12 | 1.90                     | 0.53              |
| 1:D:95:PHE:CD2   | 2:H:27:PHE:HD1    | 2.26                     | 0.53              |
| 2:E:6:CYS:H      | 2:E:16:ARG:NH1    | 2.06                     | 0.53              |
| 2:H:480:LYS:HG3  | 2:H:539:TYR:CE2   | 2.43                     | 0.53              |
| 2:G:33:VAL:HG22  | 2:G:109:PRO:HB3   | 1.89                     | 0.53              |
| 2:F:1066:VAL:HA  | 2:F:1069:VAL:HG12 | 1.90                     | 0.53              |
| 1:C:269:ASP:OD1  | 1:C:347:ARG:NE    | 2.33                     | 0.53              |
| 2:H:6:CYS:H      | 2:H:16:ARG:NH1    | 2.06                     | 0.53              |
| 2:H:802:ILE:HG23 | 2:H:807:LEU:HB3   | 1.91                     | 0.53              |
| 2:F:33:VAL:HG22  | 2:F:109:PRO:HB3   | 1.89                     | 0.53              |
| 2:G:1216:PHE:HB3 | 2:G:1218:TYR:CD2  | 2.37                     | 0.53              |
| 1:C:95:PHE:HE2   | 2:G:27:PHE:HB2    | 1.72                     | 0.53              |
| 2:E:727:LEU:HD21 | 2:E:1215:ALA:HB2  | 1.90                     | 0.53              |
| 2:G:74:ARG:HH22  | 2:G:189:VAL:HG21  | 1.74                     | 0.53              |
| 2:E:74:ARG:HH22  | 2:E:189:VAL:HG21  | 1.74                     | 0.53              |
| 2:E:495:ARG:NH1  | 2:E:1124:PHE:O    | 2.38                     | 0.53              |
| 1:A:34:ARG:NH1   | 1:A:38:LYS:HG2    | 2.24                     | 0.53              |
| 1:C:34:ARG:NH1   | 1:C:38:LYS:HG2    | 2.24                     | 0.53              |
| 2:F:295:PHE:HZ   | 2:F:383:THR:HB    | 1.73                     | 0.53              |
| 1:A:95:PHE:HE2   | 2:E:27:PHE:HB2    | 1.73                     | 0.53              |
| 1:C:161:ALA:HB1  | 1:B:167:ILE:HG21  | 1.90                     | 0.53              |
| 2:G:1032:TRP:HZ2 | 2:G:1063:TYR:HD1  | 1.57                     | 0.53              |
| 2:G:1353:TYR:OH  | 2:G:1386:SER:OG   | 2.21                     | 0.53              |
| 2:F:1032:TRP:HZ2 | 2:F:1063:TYR:HD1  | 1.57                     | 0.53              |
| 1:A:122:LEU:HD21 | 1:B:146:ILE:HG12  | 1.90                     | 0.52              |
| 2:E:480:LYS:HG3  | 2:E:539:TYR:CE2   | 2.43                     | 0.52              |
| 2:H:727:LEU:HD21 | 2:H:1215:ALA:HB2  | 1.90                     | 0.52              |
| 2:F:74:ARG:HH22  | 2:F:189:VAL:HG21  | 1.74                     | 0.52              |
| 2:F:102:HIS:HD2  | 2:F:1273:ARG:HH11 | 1.56                     | 0.52              |
| 2:F:480:LYS:HG3  | 2:F:539:TYR:CE2   | 2.43                     | 0.52              |
| 2:F:727:LEU:HD21 | 2:F:1215:ALA:HB2  | 1.90                     | 0.52              |
| 1:A:34:ARG:NH2   | 1:A:303:SER:OG    | 2.35                     | 0.52              |
| 1:C:327:SER:HA   | 1:D:45:ALA:HB3    | 1.90                     | 0.52              |
| 1:D:32:ARG:CZ    | 1:D:278:HIS:HA    | 2.39                     | 0.52              |
| 2:E:802:ILE:HG23 | 2:E:807:LEU:HB3   | 1.91                     | 0.52              |
| 2:F:6:CYS:H      | 2:F:16:ARG:NH1    | 2.06                     | 0.52              |
| 2:F:1129:ASN:OD1 | 2:F:1133:GLN:NE2  | 2.43                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:575:VAL:HG23 | 2:H:576:ALA:H     | 1.74                     | 0.52              |
| 1:C:276:HIS:HD2  | 2:G:1355:SER:CB   | 2.06                     | 0.52              |
| 1:D:273:SER:OG   | 2:H:1398:PHE:CD2  | 2.59                     | 0.52              |
| 2:H:74:ARG:HH22  | 2:H:189:VAL:HG21  | 1.74                     | 0.52              |
| 1:C:45:ALA:HB3   | 1:B:327:SER:HA    | 1.92                     | 0.52              |
| 1:C:138:VAL:O    | 1:B:136:ARG:NH2   | 2.34                     | 0.52              |
| 2:G:802:ILE:HG23 | 2:G:807:LEU:HB3   | 1.91                     | 0.52              |
| 2:G:1066:VAL:HA  | 2:G:1069:VAL:HG12 | 1.90                     | 0.52              |
| 2:F:575:VAL:HG23 | 2:F:576:ALA:H     | 1.74                     | 0.52              |
| 1:A:32:ARG:CZ    | 1:A:278:HIS:HA    | 2.40                     | 0.52              |
| 1:A:187:ALA:O    | 1:A:310:LEU:N     | 2.43                     | 0.52              |
| 1:C:50:ARG:N     | 3:B:501:ATP:N1    | 2.51                     | 0.52              |
| 2:H:593:LEU:HA   | 2:H:596:VAL:HB    | 1.92                     | 0.52              |
| 2:H:1066:VAL:HA  | 2:H:1069:VAL:HG12 | 1.90                     | 0.52              |
| 2:H:1129:ASN:OD1 | 2:H:1133:GLN:NE2  | 2.43                     | 0.52              |
| 2:H:708:LEU:O    | 2:H:897:ASP:N     | 2.40                     | 0.52              |
| 2:H:1032:TRP:HZ3 | 2:H:1067:PHE:HB2  | 1.74                     | 0.52              |
| 2:G:1129:ASN:OD1 | 2:G:1133:GLN:NE2  | 2.43                     | 0.52              |
| 1:D:187:ALA:O    | 1:D:310:LEU:N     | 2.43                     | 0.52              |
| 2:F:802:ILE:HG23 | 2:F:807:LEU:HB3   | 1.91                     | 0.52              |
| 2:G:295:PHE:HZ   | 2:G:383:THR:HB    | 1.73                     | 0.52              |
| 2:G:593:LEU:HA   | 2:G:596:VAL:HB    | 1.92                     | 0.52              |
| 2:F:495:ARG:NH1  | 2:F:1124:PHE:O    | 2.38                     | 0.52              |
| 2:E:1129:ASN:OD1 | 2:E:1133:GLN:NE2  | 2.43                     | 0.51              |
| 2:G:487:SER:HA   | 2:G:490:GLU:HG2   | 1.92                     | 0.51              |
| 2:G:575:VAL:HG23 | 2:G:576:ALA:H     | 1.74                     | 0.51              |
| 1:C:32:ARG:CZ    | 1:C:278:HIS:HA    | 2.39                     | 0.51              |
| 1:D:184:SER:OG   | 1:D:186:HIS:O     | 2.24                     | 0.51              |
| 2:G:412:MET:HA   | 2:G:416:GLN:NE2   | 2.26                     | 0.51              |
| 2:G:465:ALA:HA   | 2:G:468:ILE:HD12  | 1.93                     | 0.51              |
| 2:F:1353:TYR:OH  | 2:F:1386:SER:OG   | 2.22                     | 0.51              |
| 1:A:327:SER:HA   | 1:B:45:ALA:HB3    | 1.92                     | 0.51              |
| 1:B:187:ALA:O    | 1:B:310:LEU:N     | 2.43                     | 0.51              |
| 2:E:465:ALA:HA   | 2:E:468:ILE:HD12  | 1.93                     | 0.51              |
| 2:E:1032:TRP:HZ3 | 2:E:1067:PHE:HB2  | 1.75                     | 0.51              |
| 2:H:846:HIS:O    | 2:H:846:HIS:ND1   | 2.44                     | 0.51              |
| 2:G:1269:ASN:O   | 2:G:1273:ARG:N    | 2.29                     | 0.51              |
| 2:F:487:SER:HA   | 2:F:490:GLU:HG2   | 1.92                     | 0.51              |
| 2:F:739:TRP:CE3  | 2:F:766:ARG:HA    | 2.42                     | 0.51              |
| 1:C:184:SER:OG   | 1:C:186:HIS:O     | 2.23                     | 0.51              |
| 1:C:187:ALA:O    | 1:C:310:LEU:N     | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:846:HIS:O     | 2:E:846:HIS:ND1   | 2.44                     | 0.51              |
| 1:A:271:ALA:HB2   | 1:A:345:THR:HG22  | 1.93                     | 0.51              |
| 1:C:34:ARG:NH2    | 1:C:303:SER:OG    | 2.35                     | 0.51              |
| 2:E:451:LEU:O     | 2:E:455:ILE:HG22  | 2.11                     | 0.51              |
| 2:H:1032:TRP:HZ2  | 2:H:1063:TYR:HD1  | 1.57                     | 0.51              |
| 2:F:1032:TRP:HZ3  | 2:F:1067:PHE:HB2  | 1.75                     | 0.51              |
| 1:A:177:ARG:HG2   | 1:A:291:VAL:HG22  | 1.93                     | 0.51              |
| 1:B:32:ARG:CZ     | 1:B:278:HIS:HA    | 2.39                     | 0.51              |
| 2:E:678:CYS:HB2   | 2:E:703:ILE:O     | 2.11                     | 0.51              |
| 2:E:1032:TRP:HZ2  | 2:E:1063:TYR:HD1  | 1.57                     | 0.51              |
| 2:H:549:ALA:HB1   | 2:H:1075:ILE:HG13 | 1.93                     | 0.51              |
| 2:G:500:ASN:O     | 2:G:504:ARG:HG2   | 2.11                     | 0.51              |
| 2:F:593:LEU:HA    | 2:F:596:VAL:HB    | 1.92                     | 0.51              |
| 1:D:34:ARG:NH1    | 1:D:38:LYS:HG2    | 2.24                     | 0.51              |
| 2:E:487:SER:HA    | 2:E:490:GLU:HG2   | 1.92                     | 0.51              |
| 2:H:465:ALA:HA    | 2:H:468:ILE:HD12  | 1.93                     | 0.51              |
| 2:H:487:SER:HA    | 2:H:490:GLU:HG2   | 1.92                     | 0.51              |
| 2:G:678:CYS:HB2   | 2:G:703:ILE:O     | 2.11                     | 0.51              |
| 2:G:1011:LEU:HD11 | 2:G:1091:LYS:HD3  | 1.93                     | 0.51              |
| 2:F:537:ALA:HA    | 2:F:540:THR:HG22  | 1.93                     | 0.51              |
| 2:E:14:ALA:O      | 2:E:17:VAL:HG22   | 2.11                     | 0.51              |
| 2:E:412:MET:HA    | 2:E:416:GLN:NE2   | 2.26                     | 0.51              |
| 2:H:14:ALA:O      | 2:H:17:VAL:HG22   | 2.11                     | 0.51              |
| 2:H:412:MET:HA    | 2:H:416:GLN:NE2   | 2.26                     | 0.51              |
| 2:H:1011:LEU:HD11 | 2:H:1091:LYS:HD3  | 1.93                     | 0.51              |
| 2:H:1445:CYS:SG   | 2:H:1449:THR:OG1  | 2.54                     | 0.51              |
| 2:G:451:LEU:O     | 2:G:455:ILE:HG22  | 2.11                     | 0.51              |
| 2:F:871:GLY:O     | 2:F:875:LEU:HG    | 2.11                     | 0.51              |
| 2:F:1011:LEU:HD11 | 2:F:1091:LYS:HD3  | 1.93                     | 0.51              |
| 1:B:271:ALA:HB2   | 1:B:345:THR:HG22  | 1.93                     | 0.51              |
| 2:E:500:ASN:O     | 2:E:504:ARG:HG2   | 2.11                     | 0.51              |
| 2:H:451:LEU:O     | 2:H:455:ILE:HG22  | 2.11                     | 0.51              |
| 2:G:871:GLY:O     | 2:G:875:LEU:HG    | 2.11                     | 0.51              |
| 2:G:1032:TRP:HZ3  | 2:G:1067:PHE:HB2  | 1.75                     | 0.51              |
| 1:B:177:ARG:HG2   | 1:B:291:VAL:HG22  | 1.93                     | 0.51              |
| 1:D:314:ARG:NE    | 1:D:339:VAL:HG21  | 2.26                     | 0.51              |
| 2:E:442:PRO:HA    | 2:E:445:ILE:HG22  | 1.93                     | 0.51              |
| 2:H:678:CYS:HB2   | 2:H:703:ILE:O     | 2.11                     | 0.51              |
| 2:H:871:GLY:O     | 2:H:875:LEU:HG    | 2.11                     | 0.51              |
| 2:G:537:ALA:HA    | 2:G:540:THR:HG22  | 1.93                     | 0.51              |
| 2:F:451:LEU:O     | 2:F:455:ILE:HG22  | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:231:VAL:HB    | 1:C:234:HIS:HB2   | 1.94                     | 0.50              |
| 1:B:209:MET:O     | 1:B:292:GLU:HB2   | 2.11                     | 0.50              |
| 1:D:177:ARG:HG2   | 1:D:291:VAL:HG22  | 1.93                     | 0.50              |
| 2:E:600:THR:O     | 2:E:604:LEU:HD23  | 2.12                     | 0.50              |
| 2:E:871:GLY:O     | 2:E:875:LEU:HG    | 2.11                     | 0.50              |
| 2:E:1011:LEU:HD11 | 2:E:1091:LYS:HD3  | 1.93                     | 0.50              |
| 2:F:465:ALA:HA    | 2:F:468:ILE:HD12  | 1.93                     | 0.50              |
| 2:F:500:ASN:O     | 2:F:504:ARG:HG2   | 2.11                     | 0.50              |
| 1:C:209:MET:O     | 1:C:292:GLU:HB2   | 2.11                     | 0.50              |
| 2:E:593:LEU:HA    | 2:E:596:VAL:HB    | 1.92                     | 0.50              |
| 2:H:21:VAL:HG23   | 2:H:22:LEU:HD12   | 1.93                     | 0.50              |
| 2:G:14:ALA:O      | 2:G:17:VAL:HG22   | 2.11                     | 0.50              |
| 2:G:442:PRO:HA    | 2:G:445:ILE:HG22  | 1.94                     | 0.50              |
| 2:G:519:ARG:HD2   | 2:G:1102:ASN:OD1  | 2.12                     | 0.50              |
| 2:F:678:CYS:HB2   | 2:F:703:ILE:O     | 2.11                     | 0.50              |
| 2:F:1445:CYS:SG   | 2:F:1449:THR:OG1  | 2.54                     | 0.50              |
| 1:B:231:VAL:HB    | 1:B:234:HIS:HB2   | 1.94                     | 0.50              |
| 1:D:271:ALA:HB2   | 1:D:345:THR:HG22  | 1.93                     | 0.50              |
| 2:H:547:ASN:ND2   | 2:H:590:LEU:O     | 2.29                     | 0.50              |
| 2:H:600:THR:O     | 2:H:604:LEU:HD23  | 2.12                     | 0.50              |
| 2:G:846:HIS:O     | 2:G:846:HIS:ND1   | 2.44                     | 0.50              |
| 2:F:442:PRO:HA    | 2:F:445:ILE:HG22  | 1.94                     | 0.50              |
| 2:F:497:LYS:HA    | 2:F:500:ASN:HD22  | 1.76                     | 0.50              |
| 1:A:209:MET:O     | 1:A:292:GLU:HB2   | 2.11                     | 0.50              |
| 1:A:314:ARG:NE    | 1:A:339:VAL:HG21  | 2.26                     | 0.50              |
| 1:C:322:GLU:O     | 1:C:324:GLY:N     | 2.44                     | 0.50              |
| 2:E:1131:ILE:HA   | 2:E:1135:ILE:HD12 | 1.93                     | 0.50              |
| 2:H:1375:GLY:N    | 2:H:1547:LEU:O    | 2.45                     | 0.50              |
| 2:G:600:THR:O     | 2:G:604:LEU:HD23  | 2.12                     | 0.50              |
| 2:F:600:THR:O     | 2:F:604:LEU:HD23  | 2.12                     | 0.50              |
| 2:F:1202:HIS:HD2  | 2:F:1226:LEU:HD12 | 1.77                     | 0.50              |
| 2:F:1422:SER:HB2  | 2:F:1502:PHE:CB   | 2.42                     | 0.50              |
| 1:B:278:HIS:CD2   | 2:F:1356:SER:HG   | 2.28                     | 0.50              |
| 2:E:549:ALA:HB1   | 2:E:1075:ILE:HG13 | 1.93                     | 0.50              |
| 2:E:739:TRP:CE3   | 2:E:766:ARG:HA    | 2.42                     | 0.50              |
| 2:G:497:LYS:HA    | 2:G:500:ASN:HD22  | 1.76                     | 0.50              |
| 2:F:412:MET:HA    | 2:F:416:GLN:NE2   | 2.26                     | 0.50              |
| 2:F:846:HIS:O     | 2:F:846:HIS:ND1   | 2.44                     | 0.50              |
| 1:C:177:ARG:HG2   | 1:C:291:VAL:HG22  | 1.93                     | 0.50              |
| 1:D:209:MET:O     | 1:D:292:GLU:HB2   | 2.11                     | 0.50              |
| 1:D:335:ASN:HD22  | 1:D:336:THR:N     | 2.10                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:442:PRO:HA   | 2:H:445:ILE:HG22  | 1.94                     | 0.50              |
| 2:H:500:ASN:O    | 2:H:504:ARG:HG2   | 2.11                     | 0.50              |
| 2:H:537:ALA:HA   | 2:H:540:THR:HG22  | 1.93                     | 0.50              |
| 2:H:739:TRP:CE3  | 2:H:766:ARG:HA    | 2.43                     | 0.50              |
| 2:F:6:CYS:HB3    | 2:F:105:HIS:CD2   | 2.47                     | 0.50              |
| 1:C:314:ARG:NE   | 1:C:339:VAL:HG21  | 2.26                     | 0.50              |
| 1:B:335:ASN:HD22 | 1:B:336:THR:N     | 2.10                     | 0.50              |
| 1:D:95:PHE:HE2   | 2:H:27:PHE:HB2    | 1.76                     | 0.50              |
| 2:E:1026:LEU:O   | 2:E:1029:ILE:HG22 | 2.12                     | 0.50              |
| 2:E:1422:SER:HB2 | 2:E:1502:PHE:CB   | 2.42                     | 0.50              |
| 2:H:780:ASN:HA   | 2:H:823:GLY:HA3   | 1.94                     | 0.50              |
| 2:G:1422:SER:HB2 | 2:G:1502:PHE:CB   | 2.42                     | 0.50              |
| 2:F:549:ALA:HB1  | 2:F:1075:ILE:HG13 | 1.93                     | 0.50              |
| 1:C:59:VAL:HB    | 2:G:49:ILE:HD12   | 1.93                     | 0.50              |
| 1:D:113:SER:HA   | 1:D:115:HIS:CE1   | 2.47                     | 0.50              |
| 2:H:455:ILE:C    | 2:H:457:GLY:H     | 2.20                     | 0.50              |
| 2:H:495:ARG:NH1  | 2:H:1124:PHE:O    | 2.38                     | 0.50              |
| 2:H:1202:HIS:HD2 | 2:H:1226:LEU:HD12 | 1.77                     | 0.50              |
| 2:G:549:ALA:HB1  | 2:G:1075:ILE:HG13 | 1.93                     | 0.50              |
| 2:G:1375:GLY:N   | 2:G:1547:LEU:O    | 2.45                     | 0.50              |
| 1:C:225:SER:OG   | 1:C:229:GLU:N     | 2.45                     | 0.50              |
| 2:E:781:ALA:HA   | 2:E:821:GLN:HE22  | 1.77                     | 0.50              |
| 2:H:1131:ILE:HA  | 2:H:1135:ILE:HD12 | 1.93                     | 0.50              |
| 2:H:1392:PHE:HD1 | 2:H:1418:ARG:HG2  | 1.77                     | 0.50              |
| 2:G:117:ALA:O    | 2:G:120:SER:OG    | 2.17                     | 0.50              |
| 2:F:455:ILE:C    | 2:F:457:GLY:H     | 2.20                     | 0.50              |
| 1:A:101:ALA:HB1  | 2:E:13:ALA:O      | 2.12                     | 0.49              |
| 1:A:231:VAL:HB   | 1:A:234:HIS:HB2   | 1.94                     | 0.49              |
| 1:C:335:ASN:HD22 | 1:C:336:THR:N     | 2.10                     | 0.49              |
| 2:E:455:ILE:C    | 2:E:457:GLY:H     | 2.20                     | 0.49              |
| 2:E:537:ALA:HA   | 2:E:540:THR:HG22  | 1.93                     | 0.49              |
| 2:E:1202:HIS:HD2 | 2:E:1226:LEU:HD12 | 1.77                     | 0.49              |
| 2:H:519:ARG:HD2  | 2:H:1102:ASN:OD1  | 2.12                     | 0.49              |
| 2:F:14:ALA:O     | 2:F:17:VAL:HG22   | 2.11                     | 0.49              |
| 2:F:519:ARG:HD2  | 2:F:1102:ASN:OD1  | 2.12                     | 0.49              |
| 2:F:1026:LEU:O   | 2:F:1029:ILE:HG22 | 2.12                     | 0.49              |
| 1:C:271:ALA:HB2  | 1:C:345:THR:HG22  | 1.93                     | 0.49              |
| 1:D:225:SER:OG   | 1:D:229:GLU:N     | 2.45                     | 0.49              |
| 1:D:322:GLU:O    | 1:D:324:GLY:N     | 2.44                     | 0.49              |
| 2:E:452:LEU:HD21 | 2:E:582:LEU:HD22  | 1.95                     | 0.49              |
| 2:H:893:LEU:C    | 2:H:895:HIS:H     | 2.20                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:455:ILE:C    | 2:G:457:GLY:H     | 2.20                     | 0.49              |
| 1:A:225:SER:OG   | 1:A:229:GLU:N     | 2.45                     | 0.49              |
| 2:E:497:LYS:HA   | 2:E:500:ASN:HD22  | 1.76                     | 0.49              |
| 2:G:396:TYR:CD1  | 2:G:1226:LEU:HD13 | 2.48                     | 0.49              |
| 2:G:781:ALA:HA   | 2:G:821:GLN:HE22  | 1.77                     | 0.49              |
| 2:G:1131:ILE:HA  | 2:G:1135:ILE:HD12 | 1.93                     | 0.49              |
| 2:F:1131:ILE:HA  | 2:F:1135:ILE:HD12 | 1.93                     | 0.49              |
| 1:A:322:GLU:O    | 1:A:324:GLY:N     | 2.45                     | 0.49              |
| 1:D:177:ARG:NH1  | 1:D:206:ARG:HB2   | 2.26                     | 0.49              |
| 2:H:396:TYR:CD1  | 2:H:1226:LEU:HD13 | 2.48                     | 0.49              |
| 2:H:781:ALA:HA   | 2:H:821:GLN:HE22  | 1.77                     | 0.49              |
| 2:H:1026:LEU:O   | 2:H:1029:ILE:HG22 | 2.12                     | 0.49              |
| 2:F:780:ASN:HA   | 2:F:823:GLY:HA3   | 1.94                     | 0.49              |
| 2:F:781:ALA:HA   | 2:F:821:GLN:HE22  | 1.77                     | 0.49              |
| 2:F:893:LEU:C    | 2:F:895:HIS:H     | 2.20                     | 0.49              |
| 1:C:113:SER:HA   | 1:C:115:HIS:CE1   | 2.47                     | 0.49              |
| 1:B:75:PHE:O     | 1:B:78:SER:OG     | 2.19                     | 0.49              |
| 1:B:322:GLU:O    | 1:B:324:GLY:N     | 2.45                     | 0.49              |
| 1:D:231:VAL:HB   | 1:D:234:HIS:HB2   | 1.94                     | 0.49              |
| 2:E:21:VAL:HG23  | 2:E:22:LEU:HD12   | 1.93                     | 0.49              |
| 2:E:1392:PHE:HD1 | 2:E:1418:ARG:HG2  | 1.77                     | 0.49              |
| 2:G:1026:LEU:O   | 2:G:1029:ILE:HG22 | 2.12                     | 0.49              |
| 2:G:1202:HIS:HD2 | 2:G:1226:LEU:HD12 | 1.77                     | 0.49              |
| 1:B:314:ARG:NE   | 1:B:339:VAL:HG21  | 2.26                     | 0.49              |
| 1:D:273:SER:HG   | 2:H:1398:PHE:HD2  | 1.51                     | 0.49              |
| 2:E:519:ARG:HD2  | 2:E:1102:ASN:OD1  | 2.12                     | 0.49              |
| 2:H:452:LEU:HD21 | 2:H:582:LEU:HD22  | 1.94                     | 0.49              |
| 2:F:21:VAL:HG23  | 2:F:22:LEU:HD12   | 1.93                     | 0.49              |
| 2:F:396:TYR:CD1  | 2:F:1226:LEU:HD13 | 2.48                     | 0.49              |
| 2:F:452:LEU:HD21 | 2:F:582:LEU:HD22  | 1.94                     | 0.49              |
| 2:F:1375:GLY:N   | 2:F:1547:LEU:O    | 2.45                     | 0.49              |
| 1:A:113:SER:HA   | 1:A:115:HIS:CE1   | 2.47                     | 0.49              |
| 1:A:335:ASN:HD22 | 1:A:336:THR:N     | 2.10                     | 0.49              |
| 1:B:34:ARG:NH2   | 1:B:303:SER:OG    | 2.35                     | 0.49              |
| 1:B:113:SER:HA   | 1:B:115:HIS:CE1   | 2.47                     | 0.49              |
| 2:E:780:ASN:HA   | 2:E:823:GLY:HA3   | 1.94                     | 0.49              |
| 2:E:893:LEU:C    | 2:E:895:HIS:H     | 2.20                     | 0.49              |
| 2:H:1422:SER:HB2 | 2:H:1502:PHE:CB   | 2.42                     | 0.49              |
| 2:G:428:LEU:O    | 2:G:432:PHE:HD2   | 1.96                     | 0.49              |
| 2:G:780:ASN:HA   | 2:G:823:GLY:HA3   | 1.94                     | 0.49              |
| 2:G:1392:PHE:HD1 | 2:G:1418:ARG:HG2  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:45:ALA:HB3    | 1:D:327:SER:HA    | 1.94                     | 0.49              |
| 1:A:177:ARG:NH1   | 1:A:206:ARG:HB2   | 2.26                     | 0.49              |
| 2:E:396:TYR:CD1   | 2:E:1226:LEU:HD13 | 2.48                     | 0.49              |
| 2:H:428:LEU:O     | 2:H:432:PHE:HD2   | 1.96                     | 0.49              |
| 2:G:6:CYS:HB3     | 2:G:105:HIS:CD2   | 2.47                     | 0.49              |
| 2:G:21:VAL:HG23   | 2:G:22:LEU:HD12   | 1.93                     | 0.49              |
| 1:B:225:SER:OG    | 1:B:229:GLU:N     | 2.45                     | 0.49              |
| 2:E:6:CYS:HB3     | 2:E:105:HIS:CD2   | 2.47                     | 0.49              |
| 2:H:322:GLY:C     | 2:H:326:HIS:HD1   | 2.18                     | 0.49              |
| 2:F:713:GLY:O     | 2:F:1512:ASP:OD2  | 2.31                     | 0.49              |
| 2:E:428:LEU:O     | 2:E:432:PHE:HD2   | 1.96                     | 0.49              |
| 2:H:6:CYS:HB3     | 2:H:105:HIS:CD2   | 2.47                     | 0.49              |
| 2:F:547:ASN:ND2   | 2:F:590:LEU:O     | 2.29                     | 0.49              |
| 2:E:1423:ILE:HG13 | 2:E:1503:ILE:HG23 | 1.94                     | 0.48              |
| 2:G:739:TRP:CE3   | 2:G:766:ARG:HA    | 2.43                     | 0.48              |
| 2:G:893:LEU:C     | 2:G:895:HIS:H     | 2.20                     | 0.48              |
| 1:D:329:ASP:OD1   | 1:D:331:SER:OG    | 2.31                     | 0.48              |
| 2:E:547:ASN:HD21  | 2:E:590:LEU:C     | 2.19                     | 0.48              |
| 2:E:547:ASN:ND2   | 2:E:594:SER:HB2   | 2.26                     | 0.48              |
| 2:F:1269:ASN:O    | 2:F:1273:ARG:N    | 2.29                     | 0.48              |
| 1:A:72:LEU:HD23   | 1:B:158:MET:HE2   | 1.94                     | 0.48              |
| 1:A:344:CYS:SG    | 1:A:349:LEU:HD22  | 2.53                     | 0.48              |
| 2:E:1032:TRP:HH2  | 2:E:1063:TYR:O    | 1.96                     | 0.48              |
| 2:H:1153:LEU:HD12 | 2:H:1156:ILE:HD11 | 1.96                     | 0.48              |
| 2:F:547:ASN:ND2   | 2:F:594:SER:HB2   | 2.25                     | 0.48              |
| 1:A:95:PHE:CE1    | 2:E:16:ARG:HG2    | 2.49                     | 0.48              |
| 1:B:344:CYS:SG    | 1:B:349:LEU:HD22  | 2.53                     | 0.48              |
| 2:H:1423:ILE:HG13 | 2:H:1503:ILE:HG23 | 1.94                     | 0.48              |
| 2:F:1032:TRP:HH2  | 2:F:1063:TYR:O    | 1.96                     | 0.48              |
| 1:C:344:CYS:SG    | 1:C:349:LEU:HD22  | 2.53                     | 0.48              |
| 2:E:713:GLY:O     | 2:E:1512:ASP:OD2  | 2.31                     | 0.48              |
| 2:H:497:LYS:HA    | 2:H:500:ASN:HD22  | 1.76                     | 0.48              |
| 2:H:1275:LEU:HD12 | 2:H:1276:SER:N    | 2.29                     | 0.48              |
| 2:G:452:LEU:HD21  | 2:G:582:LEU:HD22  | 1.94                     | 0.48              |
| 2:F:428:LEU:O     | 2:F:432:PHE:HD2   | 1.96                     | 0.48              |
| 2:F:1423:ILE:HG13 | 2:F:1503:ILE:HG23 | 1.94                     | 0.48              |
| 1:D:66:LEU:HD23   | 1:D:67:LYS:N      | 2.29                     | 0.48              |
| 2:E:143:TRP:HB2   | 2:E:183:LEU:HD23  | 1.96                     | 0.48              |
| 2:H:713:GLY:O     | 2:H:1512:ASP:OD2  | 2.31                     | 0.48              |
| 1:A:244:VAL:HG22  | 1:B:239:PRO:HB3   | 1.95                     | 0.48              |
| 1:B:129:VAL:O     | 1:B:130:THR:OG1   | 2.23                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:344:CYS:SG    | 1:D:349:LEU:HD22  | 2.53                     | 0.48              |
| 2:E:453:TYR:O     | 2:E:458:VAL:HA    | 2.14                     | 0.48              |
| 2:H:143:TRP:HB2   | 2:H:183:LEU:HD23  | 1.96                     | 0.48              |
| 2:H:1375:GLY:O    | 2:H:1549:ILE:N    | 2.40                     | 0.48              |
| 2:G:1032:TRP:HH2  | 2:G:1063:TYR:O    | 1.96                     | 0.48              |
| 2:F:1392:PHE:HD1  | 2:F:1418:ARG:HG2  | 1.77                     | 0.48              |
| 1:D:34:ARG:NH2    | 1:D:303:SER:OG    | 2.35                     | 0.48              |
| 2:E:135:LEU:O     | 2:E:135:LEU:HD13  | 2.14                     | 0.48              |
| 2:G:453:TYR:O     | 2:G:458:VAL:HA    | 2.14                     | 0.48              |
| 2:G:1153:LEU:HD12 | 2:G:1156:ILE:HD11 | 1.96                     | 0.48              |
| 2:F:1275:LEU:HD12 | 2:F:1276:SER:N    | 2.29                     | 0.48              |
| 1:A:307:ASP:OD1   | 1:A:308:GLU:N     | 2.47                     | 0.48              |
| 1:C:159:ILE:O     | 1:C:163:MET:HG2   | 2.14                     | 0.48              |
| 2:H:135:LEU:HD13  | 2:H:135:LEU:O     | 2.14                     | 0.48              |
| 2:H:453:TYR:O     | 2:H:458:VAL:HA    | 2.14                     | 0.48              |
| 2:G:429:MET:HG2   | 2:G:433:PHE:CZ    | 2.49                     | 0.48              |
| 2:F:816:HIS:HB2   | 2:F:820:THR:HA    | 1.96                     | 0.48              |
| 1:C:263:ALA:HA    | 1:C:268:TYR:CG    | 2.49                     | 0.48              |
| 1:D:263:ALA:HA    | 1:D:268:TYR:CG    | 2.49                     | 0.48              |
| 1:D:307:ASP:OD1   | 1:D:308:GLU:N     | 2.47                     | 0.48              |
| 2:G:547:ASN:ND2   | 2:G:590:LEU:O     | 2.30                     | 0.48              |
| 2:G:713:GLY:O     | 2:G:1512:ASP:OD2  | 2.31                     | 0.48              |
| 1:B:307:ASP:OD1   | 1:B:308:GLU:N     | 2.47                     | 0.47              |
| 2:E:322:GLY:C     | 2:E:326:HIS:HD1   | 2.18                     | 0.47              |
| 2:H:429:MET:HG2   | 2:H:433:PHE:CZ    | 2.49                     | 0.47              |
| 2:H:1032:TRP:HH2  | 2:H:1063:TYR:O    | 1.96                     | 0.47              |
| 2:G:1275:LEU:HD12 | 2:G:1276:SER:N    | 2.29                     | 0.47              |
| 2:G:1445:CYS:SG   | 2:G:1449:THR:OG1  | 2.54                     | 0.47              |
| 2:F:143:TRP:HB2   | 2:F:183:LEU:HD23  | 1.96                     | 0.47              |
| 2:F:441:MET:HE1   | 2:F:590:LEU:HD23  | 1.96                     | 0.47              |
| 2:F:453:TYR:O     | 2:F:458:VAL:HA    | 2.14                     | 0.47              |
| 2:F:1139:LEU:O    | 2:F:1142:LEU:HD23 | 2.14                     | 0.47              |
| 1:B:94:ALA:HB2    | 1:B:114:ILE:HD11  | 1.96                     | 0.47              |
| 1:B:330:TYR:O     | 1:B:333:PHE:HB2   | 2.14                     | 0.47              |
| 2:E:1087:TRP:HA   | 2:E:1090:LEU:HD12 | 1.96                     | 0.47              |
| 2:G:135:LEU:HD13  | 2:G:135:LEU:O     | 2.14                     | 0.47              |
| 2:G:816:HIS:HB2   | 2:G:820:THR:HA    | 1.96                     | 0.47              |
| 2:G:1154:ALA:O    | 2:G:1157:SER:OG   | 2.26                     | 0.47              |
| 1:C:57:GLN:O      | 1:C:60:PHE:HB3    | 2.15                     | 0.47              |
| 1:B:66:LEU:HD23   | 1:B:67:LYS:N      | 2.29                     | 0.47              |
| 1:D:94:ALA:HB2    | 1:D:114:ILE:HD11  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1275:LEU:HD12 | 2:E:1276:SER:N    | 2.29                     | 0.47              |
| 2:H:1032:TRP:CZ3  | 2:H:1067:PHE:HB2  | 2.49                     | 0.47              |
| 2:G:143:TRP:HB2   | 2:G:183:LEU:HD23  | 1.96                     | 0.47              |
| 2:G:1423:ILE:HG13 | 2:G:1503:ILE:HG23 | 1.94                     | 0.47              |
| 1:A:76:THR:HG22   | 1:B:154:ILE:HG21  | 1.97                     | 0.47              |
| 1:A:263:ALA:HA    | 1:A:268:TYR:CG    | 2.49                     | 0.47              |
| 3:A:501:ATP:N1    | 1:B:50:ARG:N      | 2.57                     | 0.47              |
| 1:C:330:TYR:O     | 1:C:333:PHE:HB2   | 2.14                     | 0.47              |
| 1:B:57:GLN:O      | 1:B:60:PHE:HB3    | 2.14                     | 0.47              |
| 1:B:159:ILE:O     | 1:B:163:MET:HG2   | 2.14                     | 0.47              |
| 2:E:429:MET:HG2   | 2:E:433:PHE:CZ    | 2.49                     | 0.47              |
| 2:E:441:MET:HE1   | 2:E:590:LEU:HD23  | 1.96                     | 0.47              |
| 2:H:816:HIS:HB2   | 2:H:820:THR:HA    | 1.96                     | 0.47              |
| 2:G:1032:TRP:CZ3  | 2:G:1067:PHE:HB2  | 2.49                     | 0.47              |
| 2:F:1153:LEU:HD12 | 2:F:1156:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:330:TYR:O     | 1:A:333:PHE:HB2   | 2.14                     | 0.47              |
| 1:C:35:PHE:CD2    | 1:C:36:VAL:HG23   | 2.50                     | 0.47              |
| 1:C:94:ALA:HB2    | 1:C:114:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:307:ASP:OD1   | 1:C:308:GLU:N     | 2.47                     | 0.47              |
| 1:B:34:ARG:NH1    | 1:B:38:LYS:HG2    | 2.24                     | 0.47              |
| 1:B:35:PHE:CD2    | 1:B:36:VAL:HG23   | 2.50                     | 0.47              |
| 1:D:184:SER:O     | 1:D:304:TYR:OH    | 2.32                     | 0.47              |
| 2:E:547:ASN:ND2   | 2:E:590:LEU:O     | 2.29                     | 0.47              |
| 2:E:816:HIS:HB2   | 2:E:820:THR:HA    | 1.96                     | 0.47              |
| 2:H:1139:LEU:O    | 2:H:1142:LEU:HD23 | 2.14                     | 0.47              |
| 2:H:1245:ARG:NH2  | 2:H:1248:GLU:OE1  | 2.42                     | 0.47              |
| 2:G:322:GLY:C     | 2:G:326:HIS:HD1   | 2.18                     | 0.47              |
| 2:G:441:MET:HE1   | 2:G:590:LEU:HD23  | 1.96                     | 0.47              |
| 2:G:1548:VAL:HG23 | 2:G:1562:PRO:HG3  | 1.97                     | 0.47              |
| 1:A:89:ALA:O      | 1:A:93:ILE:HG12   | 2.15                     | 0.47              |
| 1:C:66:LEU:HD23   | 1:C:67:LYS:N      | 2.29                     | 0.47              |
| 1:D:330:TYR:O     | 1:D:333:PHE:HB2   | 2.14                     | 0.47              |
| 2:E:550:ILE:HD11  | 2:E:590:LEU:HD13  | 1.97                     | 0.47              |
| 2:E:1375:GLY:O    | 2:E:1549:ILE:N    | 2.40                     | 0.47              |
| 2:F:1032:TRP:CZ3  | 2:F:1067:PHE:HB2  | 2.49                     | 0.47              |
| 2:F:1087:TRP:HA   | 2:F:1090:LEU:HD12 | 1.97                     | 0.47              |
| 1:A:94:ALA:HB2    | 1:A:114:ILE:HD11  | 1.97                     | 0.47              |
| 1:A:159:ILE:O     | 1:A:163:MET:HG2   | 2.14                     | 0.47              |
| 1:C:95:PHE:CD2    | 2:G:27:PHE:HD1    | 2.32                     | 0.47              |
| 1:C:177:ARG:NH1   | 1:C:206:ARG:HB2   | 2.26                     | 0.47              |
| 2:E:798:TYR:CZ    | 2:E:802:ILE:HD11  | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1032:TRP:CZ3  | 2:E:1067:PHE:HB2  | 2.49                     | 0.47              |
| 2:E:1139:LEU:O    | 2:E:1142:LEU:HD23 | 2.14                     | 0.47              |
| 2:H:550:ILE:HD11  | 2:H:590:LEU:HD13  | 1.97                     | 0.47              |
| 2:H:798:TYR:CZ    | 2:H:802:ILE:HD11  | 2.50                     | 0.47              |
| 2:H:1269:ASN:O    | 2:H:1273:ARG:N    | 2.29                     | 0.47              |
| 2:H:1284:LEU:HD12 | 2:H:1285:THR:N    | 2.30                     | 0.47              |
| 2:F:82:LEU:HG     | 2:F:114:PHE:CE1   | 2.50                     | 0.47              |
| 2:F:429:MET:HG2   | 2:F:433:PHE:CZ    | 2.49                     | 0.47              |
| 2:F:1481:PHE:HB3  | 2:F:1485:GLN:HB2  | 1.97                     | 0.47              |
| 1:A:66:LEU:HD23   | 1:A:67:LYS:N      | 2.29                     | 0.47              |
| 1:D:201:ARG:HD2   | 1:D:315:PHE:HB3   | 1.97                     | 0.47              |
| 2:E:324:VAL:HG13  | 2:E:1277:ALA:HB1  | 1.97                     | 0.47              |
| 2:E:1166:ALA:C    | 2:E:1169:PRO:HD2  | 2.40                     | 0.47              |
| 2:H:82:LEU:HG     | 2:H:114:PHE:CE1   | 2.50                     | 0.47              |
| 2:H:441:MET:HE1   | 2:H:590:LEU:HD23  | 1.97                     | 0.47              |
| 2:H:701:ILE:HD11  | 2:H:907:ILE:HG21  | 1.97                     | 0.47              |
| 2:F:1422:SER:HB2  | 2:F:1502:PHE:HB3  | 1.96                     | 0.47              |
| 1:B:184:SER:OG    | 1:B:186:HIS:O     | 2.24                     | 0.47              |
| 1:B:263:ALA:HA    | 1:B:268:TYR:CG    | 2.49                     | 0.47              |
| 2:E:1153:LEU:HD12 | 2:E:1156:ILE:HD11 | 1.96                     | 0.47              |
| 2:E:1398:PHE:CD2  | 2:E:1399:GLU:HG2  | 2.50                     | 0.47              |
| 2:E:1481:PHE:HB3  | 2:E:1485:GLN:HB2  | 1.97                     | 0.47              |
| 2:H:85:LEU:HD11   | 2:H:113:ALA:HB3   | 1.97                     | 0.47              |
| 2:G:12:SER:C      | 2:G:15:TYR:H      | 2.22                     | 0.47              |
| 2:G:1166:ALA:C    | 2:G:1169:PRO:HD2  | 2.40                     | 0.47              |
| 2:F:135:LEU:HD13  | 2:F:135:LEU:O     | 2.14                     | 0.47              |
| 1:C:89:ALA:O      | 1:C:93:ILE:HG12   | 2.15                     | 0.47              |
| 1:D:57:GLN:O      | 1:D:60:PHE:HB3    | 2.14                     | 0.47              |
| 2:E:1422:SER:HB2  | 2:E:1502:PHE:HB3  | 1.96                     | 0.47              |
| 2:H:1422:SER:HB2  | 2:H:1502:PHE:HB3  | 1.96                     | 0.47              |
| 2:G:547:ASN:ND2   | 2:G:594:SER:HB2   | 2.25                     | 0.47              |
| 2:F:798:TYR:CZ    | 2:F:802:ILE:HD11  | 2.50                     | 0.47              |
| 2:F:1166:ALA:C    | 2:F:1169:PRO:HD2  | 2.40                     | 0.47              |
| 2:F:1398:PHE:CD2  | 2:F:1399:GLU:HG2  | 2.50                     | 0.47              |
| 1:A:95:PHE:HE1    | 2:E:16:ARG:CG     | 2.27                     | 0.46              |
| 1:A:136:ARG:HH12  | 1:B:137:MET:CG    | 2.28                     | 0.46              |
| 1:A:201:ARG:HD2   | 1:A:315:PHE:HB3   | 1.97                     | 0.46              |
| 1:B:177:ARG:NH1   | 1:B:206:ARG:HB2   | 2.26                     | 0.46              |
| 1:B:201:ARG:HD2   | 1:B:315:PHE:HB3   | 1.97                     | 0.46              |
| 2:E:82:LEU:HG     | 2:E:114:PHE:CE1   | 2.50                     | 0.46              |
| 2:E:701:ILE:HD11  | 2:E:907:ILE:HG21  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1181:PHE:CG   | 2:E:1247:LEU:HD22 | 2.51                     | 0.46              |
| 2:E:1284:LEU:HD12 | 2:E:1285:THR:N    | 2.30                     | 0.46              |
| 2:E:1446:SER:O    | 2:E:1449:THR:OG1  | 2.34                     | 0.46              |
| 2:G:701:ILE:HD11  | 2:G:907:ILE:HG21  | 1.97                     | 0.46              |
| 2:G:1181:PHE:CG   | 2:G:1247:LEU:HD22 | 2.51                     | 0.46              |
| 2:G:1284:LEU:HD12 | 2:G:1285:THR:N    | 2.30                     | 0.46              |
| 2:F:324:VAL:HG13  | 2:F:1277:ALA:HB1  | 1.97                     | 0.46              |
| 2:E:1349:LEU:HB3  | 2:E:1364:VAL:HG13 | 1.97                     | 0.46              |
| 2:H:46:ILE:HD12   | 2:H:123:TYR:OH    | 2.16                     | 0.46              |
| 2:H:1181:PHE:CG   | 2:H:1247:LEU:HD22 | 2.51                     | 0.46              |
| 2:G:1481:PHE:HB3  | 2:G:1485:GLN:HB2  | 1.97                     | 0.46              |
| 2:F:12:SER:C      | 2:F:15:TYR:H      | 2.22                     | 0.46              |
| 2:F:701:ILE:HD11  | 2:F:907:ILE:HG21  | 1.97                     | 0.46              |
| 2:F:1446:SER:O    | 2:F:1449:THR:OG1  | 2.33                     | 0.46              |
| 1:A:57:GLN:O      | 1:A:60:PHE:HB3    | 2.15                     | 0.46              |
| 1:A:344:CYS:HB2   | 1:A:348:GLN:OE1   | 2.16                     | 0.46              |
| 1:D:89:ALA:O      | 1:D:93:ILE:HG12   | 2.15                     | 0.46              |
| 1:D:159:ILE:O     | 1:D:163:MET:HG2   | 2.14                     | 0.46              |
| 2:E:1269:ASN:O    | 2:E:1273:ARG:N    | 2.29                     | 0.46              |
| 2:H:770:ALA:HA    | 2:H:1216:PHE:CE1  | 2.50                     | 0.46              |
| 2:H:1087:TRP:HA   | 2:H:1090:LEU:HD12 | 1.97                     | 0.46              |
| 2:G:85:LEU:HD11   | 2:G:113:ALA:HB3   | 1.97                     | 0.46              |
| 2:G:550:ILE:HD11  | 2:G:590:LEU:HD13  | 1.97                     | 0.46              |
| 2:G:798:TYR:CZ    | 2:G:802:ILE:HD11  | 2.50                     | 0.46              |
| 2:G:1139:LEU:O    | 2:G:1142:LEU:HD23 | 2.14                     | 0.46              |
| 1:B:344:CYS:HB2   | 1:B:348:GLN:OE1   | 2.16                     | 0.46              |
| 1:D:344:CYS:HB2   | 1:D:348:GLN:OE1   | 2.16                     | 0.46              |
| 2:E:1548:VAL:HG23 | 2:E:1562:PRO:HG3  | 1.97                     | 0.46              |
| 2:H:547:ASN:HD21  | 2:H:590:LEU:C     | 2.19                     | 0.46              |
| 2:H:1481:PHE:HB3  | 2:H:1485:GLN:HB2  | 1.97                     | 0.46              |
| 2:G:82:LEU:HG     | 2:G:114:PHE:CE1   | 2.50                     | 0.46              |
| 2:G:770:ALA:HA    | 2:G:1216:PHE:CE1  | 2.49                     | 0.46              |
| 2:F:1548:VAL:HG23 | 2:F:1562:PRO:HG3  | 1.97                     | 0.46              |
| 1:C:244:VAL:HG22  | 1:D:239:PRO:HB3   | 1.98                     | 0.46              |
| 1:D:35:PHE:CD2    | 1:D:36:VAL:HG23   | 2.50                     | 0.46              |
| 2:H:1398:PHE:CD2  | 2:H:1399:GLU:HG2  | 2.50                     | 0.46              |
| 2:G:455:ILE:C     | 2:G:456:LEU:HG    | 2.41                     | 0.46              |
| 2:G:1349:LEU:HB3  | 2:G:1364:VAL:HG13 | 1.97                     | 0.46              |
| 2:G:1375:GLY:O    | 2:G:1549:ILE:N    | 2.40                     | 0.46              |
| 2:F:379:VAL:O     | 2:F:383:THR:HG23  | 2.16                     | 0.46              |
| 2:F:550:ILE:HD11  | 2:F:590:LEU:HD13  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:201:ARG:HD2   | 1:C:315:PHE:HB3   | 1.97                     | 0.46              |
| 2:H:1548:VAL:HG23 | 2:H:1562:PRO:HG3  | 1.97                     | 0.46              |
| 2:G:153:LYS:O     | 2:G:157:PHE:HB2   | 2.16                     | 0.46              |
| 2:G:324:VAL:HG13  | 2:G:1277:ALA:HB1  | 1.97                     | 0.46              |
| 2:G:1087:TRP:HA   | 2:G:1090:LEU:HD12 | 1.96                     | 0.46              |
| 2:F:1003:TYR:CE1  | 2:F:1092:VAL:HG11 | 2.51                     | 0.46              |
| 1:A:35:PHE:CD2    | 1:A:36:VAL:HG23   | 2.50                     | 0.46              |
| 1:A:233:LEU:HD21  | 1:D:326:TYR:CZ    | 2.51                     | 0.46              |
| 1:C:184:SER:O     | 1:C:304:TYR:OH    | 2.32                     | 0.46              |
| 1:C:329:ASP:OD1   | 1:C:331:SER:OG    | 2.31                     | 0.46              |
| 2:H:12:SER:C      | 2:H:15:TYR:H      | 2.22                     | 0.46              |
| 2:H:1166:ALA:C    | 2:H:1169:PRO:HD2  | 2.40                     | 0.46              |
| 2:G:1003:TYR:CE1  | 2:G:1092:VAL:HG11 | 2.51                     | 0.46              |
| 2:G:1152:ALA:O    | 2:G:1156:ILE:HG12 | 2.16                     | 0.46              |
| 2:G:1398:PHE:CD2  | 2:G:1399:GLU:HG2  | 2.50                     | 0.46              |
| 2:F:1284:LEU:HD12 | 2:F:1285:THR:N    | 2.30                     | 0.46              |
| 1:C:218:GLN:NE2   | 1:C:235:GLN:OE1   | 2.49                     | 0.46              |
| 1:B:89:ALA:O      | 1:B:93:ILE:HG12   | 2.15                     | 0.46              |
| 2:E:46:ILE:HD12   | 2:E:123:TYR:OH    | 2.16                     | 0.46              |
| 2:E:379:VAL:O     | 2:E:383:THR:HG23  | 2.16                     | 0.46              |
| 2:E:1030:ASP:OD2  | 2:E:1286:TYR:OH   | 2.32                     | 0.46              |
| 2:E:1375:GLY:N    | 2:E:1547:LEU:O    | 2.45                     | 0.46              |
| 2:H:379:VAL:O     | 2:H:383:THR:HG23  | 2.16                     | 0.46              |
| 2:H:1349:LEU:HB3  | 2:H:1364:VAL:HG13 | 1.97                     | 0.46              |
| 2:H:1446:SER:O    | 2:H:1449:THR:OG1  | 2.34                     | 0.46              |
| 2:G:127:ILE:O     | 2:G:131:ASN:N     | 2.45                     | 0.46              |
| 2:G:547:ASN:HD21  | 2:G:590:LEU:C     | 2.19                     | 0.46              |
| 2:G:1379:ARG:O    | 2:G:1384:LYS:NZ   | 2.49                     | 0.46              |
| 2:F:108:MET:N     | 2:F:109:PRO:HD2   | 2.31                     | 0.46              |
| 2:F:494:GLU:O     | 2:F:498:GLN:HG2   | 2.16                     | 0.46              |
| 2:F:1181:PHE:CG   | 2:F:1247:LEU:HD22 | 2.50                     | 0.46              |
| 2:F:1568:ARG:C    | 2:F:1570:ASP:H    | 2.24                     | 0.46              |
| 1:A:218:GLN:NE2   | 1:A:235:GLN:OE1   | 2.49                     | 0.46              |
| 2:E:12:SER:C      | 2:E:15:TYR:H      | 2.22                     | 0.46              |
| 2:E:1231:ASP:O    | 2:E:1235:ILE:HG12 | 2.16                     | 0.46              |
| 2:H:148:ILE:O     | 2:H:151:THR:OG1   | 2.34                     | 0.46              |
| 2:H:324:VAL:HG13  | 2:H:1277:ALA:HB1  | 1.97                     | 0.46              |
| 2:H:461:LEU:HD12  | 2:H:461:LEU:O     | 2.16                     | 0.46              |
| 2:H:494:GLU:O     | 2:H:498:GLN:HG2   | 2.16                     | 0.46              |
| 2:H:547:ASN:ND2   | 2:H:594:SER:HB2   | 2.26                     | 0.46              |
| 2:G:379:VAL:O     | 2:G:383:THR:HG23  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:1231:ASP:O   | 2:G:1235:ILE:HG12 | 2.16                     | 0.46              |
| 2:F:45:PRO:O     | 2:F:49:ILE:HG23   | 2.16                     | 0.46              |
| 1:C:344:CYS:HB2  | 1:C:348:GLN:OE1   | 2.16                     | 0.46              |
| 2:E:85:LEU:HD11  | 2:E:113:ALA:HB3   | 1.97                     | 0.46              |
| 2:H:45:PRO:O     | 2:H:49:ILE:HG23   | 2.16                     | 0.46              |
| 2:H:1152:ALA:O   | 2:H:1156:ILE:HG12 | 2.16                     | 0.46              |
| 2:G:108:MET:N    | 2:G:109:PRO:HD2   | 2.31                     | 0.46              |
| 2:F:547:ASN:HD21 | 2:F:590:LEU:C     | 2.19                     | 0.46              |
| 1:C:72:LEU:HD23  | 1:D:158:MET:HE2   | 1.98                     | 0.45              |
| 1:C:194:GLY:N    | 1:D:227:GLU:OE2   | 2.24                     | 0.45              |
| 1:C:200:LEU:HD21 | 1:C:285:VAL:HG21  | 1.98                     | 0.45              |
| 1:B:218:GLN:NE2  | 1:B:235:GLN:OE1   | 2.49                     | 0.45              |
| 2:E:45:PRO:O     | 2:E:49:ILE:HG23   | 2.16                     | 0.45              |
| 2:H:455:ILE:C    | 2:H:456:LEU:HG    | 2.41                     | 0.45              |
| 2:H:681:ILE:HG12 | 2:H:737:VAL:HG22  | 1.98                     | 0.45              |
| 2:G:1422:SER:HB2 | 2:G:1502:PHE:HB3  | 1.96                     | 0.45              |
| 2:G:1431:PHE:HB2 | 2:G:1438:ASN:ND2  | 2.31                     | 0.45              |
| 2:F:681:ILE:HG12 | 2:F:737:VAL:HG22  | 1.98                     | 0.45              |
| 2:E:108:MET:N    | 2:E:109:PRO:HD2   | 2.31                     | 0.45              |
| 2:H:108:MET:N    | 2:H:109:PRO:HD2   | 2.31                     | 0.45              |
| 2:H:1372:GLN:HA  | 2:H:1530:ARG:O    | 2.17                     | 0.45              |
| 2:H:1431:PHE:HB2 | 2:H:1438:ASN:ND2  | 2.31                     | 0.45              |
| 2:G:45:PRO:O     | 2:G:49:ILE:HG23   | 2.16                     | 0.45              |
| 2:F:46:ILE:HD12  | 2:F:123:TYR:OH    | 2.16                     | 0.45              |
| 2:F:85:LEU:HD11  | 2:F:113:ALA:HB3   | 1.97                     | 0.45              |
| 2:F:153:LYS:O    | 2:F:157:PHE:HB2   | 2.16                     | 0.45              |
| 2:F:322:GLY:C    | 2:F:326:HIS:HD1   | 2.18                     | 0.45              |
| 2:F:1231:ASP:O   | 2:F:1235:ILE:HG12 | 2.16                     | 0.45              |
| 2:F:1379:ARG:O   | 2:F:1384:LYS:NZ   | 2.49                     | 0.45              |
| 1:B:200:LEU:HD21 | 1:B:285:VAL:HG21  | 1.98                     | 0.45              |
| 2:E:153:LYS:O    | 2:E:157:PHE:HB2   | 2.16                     | 0.45              |
| 2:E:1152:ALA:O   | 2:E:1156:ILE:HG12 | 2.16                     | 0.45              |
| 2:H:1568:ARG:C   | 2:H:1570:ASP:H    | 2.24                     | 0.45              |
| 1:D:218:GLN:NE2  | 1:D:235:GLN:OE1   | 2.49                     | 0.45              |
| 2:E:1003:TYR:CE1 | 2:E:1092:VAL:HG11 | 2.51                     | 0.45              |
| 2:H:1231:ASP:O   | 2:H:1235:ILE:HG12 | 2.16                     | 0.45              |
| 2:G:461:LEU:HD12 | 2:G:461:LEU:O     | 2.16                     | 0.45              |
| 2:G:1446:SER:O   | 2:G:1449:THR:OG1  | 2.34                     | 0.45              |
| 2:F:1152:ALA:O   | 2:F:1156:ILE:HG12 | 2.16                     | 0.45              |
| 2:F:1431:PHE:HB2 | 2:F:1438:ASN:ND2  | 2.31                     | 0.45              |
| 1:C:199:MET:HG2  | 1:C:258:TYR:HB3   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:233:LEU:HD21 | 1:B:326:TYR:CZ    | 2.51                     | 0.45              |
| 1:C:299:GLN:NE2  | 1:C:301:ARG:HD2   | 2.32                     | 0.45              |
| 2:E:1431:PHE:HB2 | 2:E:1438:ASN:ND2  | 2.31                     | 0.45              |
| 2:G:1568:ARG:C   | 2:G:1570:ASP:H    | 2.24                     | 0.45              |
| 2:E:32:ASN:ND2   | 2:E:153:LYS:HD2   | 2.32                     | 0.45              |
| 2:E:455:ILE:C    | 2:E:456:LEU:HG    | 2.41                     | 0.45              |
| 2:E:1151:SER:O   | 2:E:1155:VAL:HG23 | 2.17                     | 0.45              |
| 2:H:153:LYS:O    | 2:H:157:PHE:HB2   | 2.16                     | 0.45              |
| 2:H:1003:TYR:CE1 | 2:H:1092:VAL:HG11 | 2.51                     | 0.45              |
| 2:H:1023:HIS:HE1 | 2:H:1144:ARG:HA   | 1.82                     | 0.45              |
| 2:G:32:ASN:ND2   | 2:G:153:LYS:HD2   | 2.32                     | 0.45              |
| 2:G:46:ILE:HD12  | 2:G:123:TYR:OH    | 2.16                     | 0.45              |
| 2:G:681:ILE:HG12 | 2:G:737:VAL:HG22  | 1.98                     | 0.45              |
| 2:F:788:ILE:HG22 | 2:F:791:SER:H     | 1.82                     | 0.45              |
| 2:F:1072:SER:O   | 2:F:1075:ILE:HG22 | 2.17                     | 0.45              |
| 2:F:1181:PHE:CD2 | 2:F:1247:LEU:HD22 | 2.52                     | 0.45              |
| 1:A:299:GLN:NE2  | 1:A:301:ARG:HD2   | 2.32                     | 0.45              |
| 1:B:346:ALA:HA   | 1:B:349:LEU:HB2   | 1.99                     | 0.45              |
| 1:D:199:MET:HG2  | 1:D:258:TYR:HB3   | 1.99                     | 0.45              |
| 2:E:788:ILE:HG22 | 2:E:791:SER:H     | 1.82                     | 0.45              |
| 2:G:716:GLY:N    | 3:G:2004:ATP:O2G  | 2.34                     | 0.45              |
| 2:F:455:ILE:C    | 2:F:456:LEU:HG    | 2.41                     | 0.45              |
| 1:C:346:ALA:HA   | 1:C:349:LEU:HB2   | 1.99                     | 0.45              |
| 1:B:299:GLN:NE2  | 1:B:301:ARG:HD2   | 2.32                     | 0.45              |
| 1:D:68:TRP:CD2   | 1:D:170:LYS:HE3   | 2.52                     | 0.45              |
| 1:D:128:GLN:HB2  | 1:D:152:GLN:HE21  | 1.82                     | 0.45              |
| 2:H:1151:SER:O   | 2:H:1155:VAL:HG23 | 2.17                     | 0.45              |
| 2:G:1023:HIS:HE1 | 2:G:1144:ARG:HA   | 1.82                     | 0.45              |
| 2:F:291:LEU:O    | 2:F:295:PHE:HB3   | 2.16                     | 0.45              |
| 2:F:1502:PHE:HE2 | 2:F:1504:MET:HE3  | 1.82                     | 0.45              |
| 1:D:129:VAL:O    | 1:D:130:THR:OG1   | 2.23                     | 0.45              |
| 2:E:461:LEU:HD12 | 2:E:461:LEU:O     | 2.16                     | 0.45              |
| 2:E:494:GLU:O    | 2:E:498:GLN:HG2   | 2.16                     | 0.45              |
| 2:H:1310:ALA:HA  | 2:H:1313:ARG:NH2  | 2.32                     | 0.45              |
| 2:G:807:LEU:HG   | 2:G:811:ILE:HG13  | 1.99                     | 0.45              |
| 2:G:1245:ARG:NH2 | 2:G:1248:GLU:OE1  | 2.42                     | 0.45              |
| 2:F:1349:LEU:HB3 | 2:F:1364:VAL:HG13 | 1.97                     | 0.45              |
| 1:A:90:TRP:CE2   | 1:A:123:PHE:HE2   | 2.35                     | 0.45              |
| 1:A:269:ASP:OD1  | 1:A:347:ARG:NE    | 2.33                     | 0.45              |
| 1:C:268:TYR:CZ   | 1:C:347:ARG:HA    | 2.52                     | 0.45              |
| 1:D:200:LEU:HD21 | 1:D:285:VAL:HG21  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:294:THR:OG1   | 1:D:296:ILE:HG12  | 2.17                     | 0.45              |
| 2:E:1023:HIS:HE1  | 2:E:1144:ARG:HA   | 1.82                     | 0.45              |
| 2:E:1372:GLN:HA   | 2:E:1530:ARG:O    | 2.17                     | 0.45              |
| 2:H:1181:PHE:CD2  | 2:H:1247:LEU:HD22 | 2.52                     | 0.45              |
| 2:H:1379:ARG:O    | 2:H:1384:LYS:NZ   | 2.49                     | 0.45              |
| 2:G:1181:PHE:CD2  | 2:G:1247:LEU:HD22 | 2.52                     | 0.45              |
| 2:F:1151:SER:O    | 2:F:1155:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:68:TRP:CD2    | 1:A:170:LYS:HE3   | 2.52                     | 0.44              |
| 1:B:268:TYR:CZ    | 1:B:347:ARG:HA    | 2.52                     | 0.44              |
| 1:B:294:THR:OG1   | 1:B:296:ILE:HG12  | 2.17                     | 0.44              |
| 1:D:90:TRP:CE2    | 1:D:123:PHE:HE2   | 2.36                     | 0.44              |
| 2:E:1072:SER:O    | 2:E:1075:ILE:HG22 | 2.17                     | 0.44              |
| 2:E:1568:ARG:C    | 2:E:1570:ASP:H    | 2.24                     | 0.44              |
| 2:H:1072:SER:O    | 2:H:1075:ILE:HG22 | 2.17                     | 0.44              |
| 2:G:771:TYR:HD2   | 2:G:1212:THR:HG22 | 1.82                     | 0.44              |
| 2:G:1351:VAL:HG12 | 2:G:1397:THR:HA   | 1.99                     | 0.44              |
| 2:G:1372:GLN:HA   | 2:G:1530:ARG:O    | 2.17                     | 0.44              |
| 2:F:1271:LEU:HG   | 2:F:1272:HIS:CD2  | 2.52                     | 0.44              |
| 1:A:200:LEU:HD21  | 1:A:285:VAL:HG21  | 1.98                     | 0.44              |
| 1:D:95:PHE:HD2    | 2:H:27:PHE:HD1    | 1.65                     | 0.44              |
| 1:D:268:TYR:CZ    | 1:D:347:ARG:HA    | 2.52                     | 0.44              |
| 2:E:291:LEU:O     | 2:E:295:PHE:HB3   | 2.17                     | 0.44              |
| 2:E:1271:LEU:HG   | 2:E:1272:HIS:CD2  | 2.52                     | 0.44              |
| 2:H:1351:VAL:HG12 | 2:H:1397:THR:HA   | 2.00                     | 0.44              |
| 2:G:36:HIS:HD2    | 2:G:142:TYR:HE1   | 1.66                     | 0.44              |
| 2:G:291:LEU:O     | 2:G:295:PHE:HB3   | 2.16                     | 0.44              |
| 2:G:494:GLU:O     | 2:G:498:GLN:HG2   | 2.16                     | 0.44              |
| 2:G:788:ILE:HG22  | 2:G:791:SER:H     | 1.82                     | 0.44              |
| 2:G:1502:PHE:HE2  | 2:G:1504:MET:HE3  | 1.82                     | 0.44              |
| 2:F:381:ILE:HG13  | 2:F:433:PHE:CZ    | 2.53                     | 0.44              |
| 2:F:417:ILE:O     | 2:F:420:LEU:HG    | 2.18                     | 0.44              |
| 2:F:461:LEU:O     | 2:F:461:LEU:HD12  | 2.16                     | 0.44              |
| 2:F:1310:ALA:HA   | 2:F:1313:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:268:TYR:CZ    | 1:A:347:ARG:HA    | 2.52                     | 0.44              |
| 1:B:286:ILE:HG23  | 1:B:299:GLN:HE21  | 1.83                     | 0.44              |
| 1:D:299:GLN:NE2   | 1:D:301:ARG:HD2   | 2.32                     | 0.44              |
| 2:E:1181:PHE:CD2  | 2:E:1247:LEU:HD22 | 2.52                     | 0.44              |
| 2:G:32:ASN:HD21   | 2:G:153:LYS:HD2   | 1.83                     | 0.44              |
| 2:G:1151:SER:O    | 2:G:1155:VAL:HG23 | 2.17                     | 0.44              |
| 2:F:771:TYR:HD2   | 2:F:1212:THR:HG22 | 1.82                     | 0.44              |
| 2:F:1023:HIS:HE1  | 2:F:1144:ARG:HA   | 1.82                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:278:HIS:ND1  | 2:E:1355:SER:OG   | 2.47                     | 0.44              |
| 1:C:76:THR:HG22  | 1:D:154:ILE:HG21  | 1.99                     | 0.44              |
| 1:C:294:THR:OG1  | 1:C:296:ILE:HG12  | 2.17                     | 0.44              |
| 1:B:68:TRP:CD2   | 1:B:170:LYS:HE3   | 2.52                     | 0.44              |
| 1:B:128:GLN:HB2  | 1:B:152:GLN:HE21  | 1.82                     | 0.44              |
| 2:E:417:ILE:O    | 2:E:420:LEU:HG    | 2.18                     | 0.44              |
| 2:E:807:LEU:HG   | 2:E:811:ILE:HG13  | 1.99                     | 0.44              |
| 2:H:291:LEU:O    | 2:H:295:PHE:HB3   | 2.17                     | 0.44              |
| 2:G:381:ILE:HG13 | 2:G:433:PHE:CZ    | 2.53                     | 0.44              |
| 2:G:889:LYS:NZ   | 2:G:892:TYR:HE2   | 2.16                     | 0.44              |
| 2:G:1310:ALA:HA  | 2:G:1313:ARG:NH2  | 2.32                     | 0.44              |
| 2:F:36:HIS:HD2   | 2:F:142:TYR:HE1   | 1.66                     | 0.44              |
| 2:F:889:LYS:NZ   | 2:F:892:TYR:HE2   | 2.16                     | 0.44              |
| 2:F:1245:ARG:NH2 | 2:F:1248:GLU:OE1  | 2.42                     | 0.44              |
| 2:F:1348:ASN:O   | 2:F:1350:SER:N    | 2.49                     | 0.44              |
| 2:F:1372:GLN:HA  | 2:F:1530:ARG:O    | 2.17                     | 0.44              |
| 1:A:164:LEU:HD11 | 1:B:164:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:199:MET:HG2  | 1:A:258:TYR:HB3   | 1.99                     | 0.44              |
| 1:C:68:TRP:CD2   | 1:C:170:LYS:HE3   | 2.52                     | 0.44              |
| 1:D:286:ILE:HG23 | 1:D:299:GLN:HE21  | 1.82                     | 0.44              |
| 2:E:36:HIS:HD2   | 2:E:142:TYR:HE1   | 1.66                     | 0.44              |
| 2:E:471:ALA:HB3  | 2:E:472:PRO:HD3   | 2.00                     | 0.44              |
| 2:E:889:LYS:NZ   | 2:E:892:TYR:HE2   | 2.16                     | 0.44              |
| 2:E:1348:ASN:O   | 2:E:1350:SER:N    | 2.49                     | 0.44              |
| 2:H:771:TYR:HD2  | 2:H:1212:THR:HG22 | 1.82                     | 0.44              |
| 2:G:417:ILE:O    | 2:G:420:LEU:HG    | 2.18                     | 0.44              |
| 2:G:1455:GLU:OE1 | 2:G:1460:LYS:HB3  | 2.18                     | 0.44              |
| 2:F:32:ASN:ND2   | 2:F:153:LYS:HD2   | 2.32                     | 0.44              |
| 2:F:770:ALA:HA   | 2:F:1216:PHE:CE1  | 2.50                     | 0.44              |
| 1:A:294:THR:OG1  | 1:A:296:ILE:HG12  | 2.17                     | 0.44              |
| 1:B:329:ASP:OD1  | 1:B:331:SER:OG    | 2.31                     | 0.44              |
| 2:E:32:ASN:HD21  | 2:E:153:LYS:HD2   | 1.83                     | 0.44              |
| 2:E:681:ILE:HG12 | 2:E:737:VAL:HG22  | 1.98                     | 0.44              |
| 2:E:1066:VAL:O   | 2:E:1069:VAL:HG12 | 2.18                     | 0.44              |
| 2:H:36:HIS:HD2   | 2:H:142:TYR:HE1   | 1.66                     | 0.44              |
| 2:H:471:ALA:HB3  | 2:H:472:PRO:HD3   | 2.00                     | 0.44              |
| 2:H:788:ILE:HG22 | 2:H:791:SER:H     | 1.82                     | 0.44              |
| 2:H:1376:ILE:HB  | 2:H:1535:ILE:HD13 | 2.00                     | 0.44              |
| 2:G:1348:ASN:O   | 2:G:1350:SER:N    | 2.49                     | 0.44              |
| 2:F:1455:GLU:OE1 | 2:F:1460:LYS:HB3  | 2.18                     | 0.44              |
| 1:A:128:GLN:HB2  | 1:A:152:GLN:HE21  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:1455:GLU:OE1 | 2:E:1460:LYS:HB3  | 2.18                     | 0.44              |
| 2:H:1066:VAL:O   | 2:H:1069:VAL:HG12 | 2.18                     | 0.44              |
| 2:F:32:ASN:HD21  | 2:F:153:LYS:HD2   | 1.83                     | 0.44              |
| 1:A:346:ALA:HA   | 1:A:349:LEU:HB2   | 1.99                     | 0.44              |
| 1:C:90:TRP:CE2   | 1:C:123:PHE:HE2   | 2.36                     | 0.44              |
| 1:C:286:ILE:HG23 | 1:C:299:GLN:HE21  | 1.82                     | 0.44              |
| 1:B:199:MET:HG2  | 1:B:258:TYR:HB3   | 1.99                     | 0.44              |
| 1:D:199:MET:HG2  | 1:D:258:TYR:CB    | 2.48                     | 0.44              |
| 2:H:32:ASN:ND2   | 2:H:153:LYS:HD2   | 2.32                     | 0.44              |
| 2:H:435:CYS:N    | 2:H:436:PRO:HD2   | 2.33                     | 0.44              |
| 2:H:807:LEU:HG   | 2:H:811:ILE:HG13  | 1.99                     | 0.44              |
| 2:G:437:ASN:ND2  | 2:G:592:LEU:HD23  | 2.29                     | 0.44              |
| 1:A:286:ILE:HG23 | 1:A:299:GLN:HE21  | 1.82                     | 0.44              |
| 1:C:126:GLU:OE2  | 1:C:136:ARG:NH1   | 2.51                     | 0.44              |
| 1:C:229:GLU:HB3  | 1:B:314:ARG:CZ    | 2.48                     | 0.44              |
| 2:E:127:ILE:O    | 2:E:131:ASN:N     | 2.45                     | 0.44              |
| 2:E:381:ILE:HG13 | 2:E:433:PHE:CZ    | 2.53                     | 0.44              |
| 2:H:32:ASN:HD21  | 2:H:153:LYS:HD2   | 1.83                     | 0.44              |
| 2:G:127:ILE:HG23 | 2:G:128:GLU:N     | 2.33                     | 0.44              |
| 2:G:1066:VAL:O   | 2:G:1069:VAL:HG12 | 2.18                     | 0.44              |
| 2:F:1460:LYS:O   | 2:F:1464:LYS:HG2  | 2.18                     | 0.44              |
| 1:D:126:GLU:OE2  | 1:D:136:ARG:NH1   | 2.51                     | 0.43              |
| 2:E:1379:ARG:O   | 2:E:1384:LYS:NZ   | 2.49                     | 0.43              |
| 2:H:127:ILE:O    | 2:H:131:ASN:N     | 2.45                     | 0.43              |
| 2:H:127:ILE:HG23 | 2:H:128:GLU:N     | 2.33                     | 0.43              |
| 2:H:141:VAL:O    | 2:H:144:THR:OG1   | 2.32                     | 0.43              |
| 2:G:1271:LEU:HG  | 2:G:1272:HIS:CD2  | 2.52                     | 0.43              |
| 2:F:807:LEU:HG   | 2:F:811:ILE:HG13  | 1.99                     | 0.43              |
| 1:A:119:SER:OG   | 1:B:140:GLU:OE2   | 2.17                     | 0.43              |
| 1:C:190:ALA:O    | 1:C:196:LEU:HD12  | 2.18                     | 0.43              |
| 1:C:199:MET:HG2  | 1:C:258:TYR:CB    | 2.48                     | 0.43              |
| 1:B:269:ASP:OD1  | 1:B:347:ARG:NE    | 2.33                     | 0.43              |
| 1:D:346:ALA:HA   | 1:D:349:LEU:HB2   | 1.99                     | 0.43              |
| 2:E:1502:PHE:HE2 | 2:E:1504:MET:HE3  | 1.82                     | 0.43              |
| 2:G:302:SER:OG   | 2:G:376:SER:O     | 2.31                     | 0.43              |
| 2:G:1376:ILE:HB  | 2:G:1535:ILE:HD13 | 2.00                     | 0.43              |
| 2:G:1460:LYS:O   | 2:G:1464:LYS:HG2  | 2.19                     | 0.43              |
| 2:F:1030:ASP:OD2 | 2:F:1286:TYR:OH   | 2.32                     | 0.43              |
| 1:B:190:ALA:O    | 1:B:196:LEU:HD12  | 2.18                     | 0.43              |
| 1:B:199:MET:HG2  | 1:B:258:TYR:CB    | 2.48                     | 0.43              |
| 2:E:1310:ALA:HA  | 2:E:1313:ARG:NH2  | 2.32                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:417:ILE:O     | 2:H:420:LEU:HG    | 2.18                     | 0.43              |
| 2:H:1180:TYR:O    | 2:H:1183:VAL:HG12 | 2.19                     | 0.43              |
| 2:G:1180:TYR:O    | 2:G:1183:VAL:HG12 | 2.19                     | 0.43              |
| 2:F:1351:VAL:HG12 | 2:F:1397:THR:HA   | 1.99                     | 0.43              |
| 1:A:199:MET:HG2   | 1:A:258:TYR:CB    | 2.48                     | 0.43              |
| 1:D:122:LEU:O     | 1:D:126:GLU:HG3   | 2.19                     | 0.43              |
| 1:D:190:ALA:O     | 1:D:196:LEU:HD12  | 2.18                     | 0.43              |
| 2:E:148:ILE:O     | 2:E:151:THR:OG1   | 2.34                     | 0.43              |
| 2:E:721:SER:HB3   | 2:E:730:MET:HE1   | 2.00                     | 0.43              |
| 2:E:1351:VAL:HG12 | 2:E:1397:THR:HA   | 1.99                     | 0.43              |
| 2:E:1376:ILE:HB   | 2:E:1535:ILE:HD13 | 2.00                     | 0.43              |
| 2:H:309:ALA:HB1   | 2:H:369:GLN:OE1   | 2.19                     | 0.43              |
| 2:H:1271:LEU:HG   | 2:H:1272:HIS:CD2  | 2.52                     | 0.43              |
| 2:H:1460:LYS:O    | 2:H:1464:LYS:HG2  | 2.18                     | 0.43              |
| 2:G:471:ALA:HB3   | 2:G:472:PRO:HD3   | 2.00                     | 0.43              |
| 2:G:1072:SER:O    | 2:G:1075:ILE:HG22 | 2.17                     | 0.43              |
| 2:G:1491:LEU:HD11 | 2:G:1507:ALA:HB1  | 2.00                     | 0.43              |
| 2:F:1130:THR:O    | 2:F:1134:HIS:HB2  | 2.19                     | 0.43              |
| 1:B:90:TRP:CE2    | 1:B:123:PHE:HE2   | 2.36                     | 0.43              |
| 1:B:184:SER:O     | 1:B:304:TYR:OH    | 2.32                     | 0.43              |
| 1:D:200:LEU:HD22  | 1:D:304:TYR:CE2   | 2.54                     | 0.43              |
| 2:E:302:SER:OG    | 2:E:376:SER:O     | 2.31                     | 0.43              |
| 2:H:381:ILE:HG13  | 2:H:433:PHE:CZ    | 2.53                     | 0.43              |
| 2:H:521:ARG:O     | 2:H:524:THR:OG1   | 2.36                     | 0.43              |
| 2:G:39:LEU:HA     | 2:G:42:ILE:HG22   | 2.01                     | 0.43              |
| 2:F:309:ALA:HB1   | 2:F:369:GLN:OE1   | 2.19                     | 0.43              |
| 2:F:314:PHE:HZ    | 2:F:448:GLY:HA2   | 1.83                     | 0.43              |
| 2:F:1154:ALA:O    | 2:F:1157:SER:OG   | 2.26                     | 0.43              |
| 1:A:126:GLU:OE2   | 1:A:136:ARG:NH1   | 2.51                     | 0.43              |
| 1:C:128:GLN:HB2   | 1:C:152:GLN:HE21  | 1.82                     | 0.43              |
| 1:B:126:GLU:OE2   | 1:B:136:ARG:NH1   | 2.51                     | 0.43              |
| 2:E:552:ILE:HA    | 2:E:555:VAL:HG22  | 2.01                     | 0.43              |
| 2:G:521:ARG:O     | 2:G:524:THR:OG1   | 2.36                     | 0.43              |
| 2:G:771:TYR:HD1   | 2:G:851:PHE:HD2   | 1.66                     | 0.43              |
| 2:F:127:ILE:O     | 2:F:131:ASN:N     | 2.45                     | 0.43              |
| 2:F:435:CYS:N     | 2:F:436:PRO:HD2   | 2.33                     | 0.43              |
| 2:F:1066:VAL:O    | 2:F:1069:VAL:HG12 | 2.18                     | 0.43              |
| 2:F:1491:LEU:HD11 | 2:F:1507:ALA:HB1  | 1.99                     | 0.43              |
| 1:A:122:LEU:O     | 1:A:126:GLU:HG3   | 2.19                     | 0.43              |
| 2:E:127:ILE:HG23  | 2:E:128:GLU:N     | 2.33                     | 0.43              |
| 2:E:1130:THR:O    | 2:E:1134:HIS:HB2  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1491:LEU:HD11 | 2:E:1507:ALA:HB1  | 1.99                     | 0.43              |
| 2:H:889:LYS:NZ    | 2:H:892:TYR:HE2   | 2.16                     | 0.43              |
| 2:H:1130:THR:O    | 2:H:1134:HIS:HB2  | 2.19                     | 0.43              |
| 2:H:1491:LEU:HD11 | 2:H:1507:ALA:HB1  | 1.99                     | 0.43              |
| 2:G:721:SER:HB3   | 2:G:730:MET:HE1   | 2.00                     | 0.43              |
| 2:F:471:ALA:HB3   | 2:F:472:PRO:HD3   | 2.00                     | 0.43              |
| 1:A:108:GLU:OE1   | 1:A:108:GLU:N     | 2.52                     | 0.43              |
| 1:A:190:ALA:O     | 1:A:196:LEU:HD12  | 2.18                     | 0.43              |
| 1:C:108:GLU:N     | 1:C:108:GLU:OE1   | 2.52                     | 0.43              |
| 1:C:200:LEU:HD22  | 1:C:304:TYR:CE2   | 2.54                     | 0.43              |
| 2:E:39:LEU:HA     | 2:E:42:ILE:HG22   | 2.01                     | 0.43              |
| 2:E:771:TYR:HD1   | 2:E:851:PHE:HD2   | 1.66                     | 0.43              |
| 2:H:39:LEU:HA     | 2:H:42:ILE:HG22   | 2.01                     | 0.43              |
| 2:H:395:ILE:HG21  | 2:H:421:VAL:HG12  | 2.01                     | 0.43              |
| 2:H:890:LEU:O     | 2:H:893:LEU:HG    | 2.19                     | 0.43              |
| 2:H:1502:PHE:HE2  | 2:H:1504:MET:HE3  | 1.82                     | 0.43              |
| 1:C:286:ILE:HD13  | 1:B:250:PHE:CD1   | 2.54                     | 0.43              |
| 1:B:242:ASN:OD1   | 1:B:243:GLY:N     | 2.52                     | 0.43              |
| 2:E:309:ALA:HB1   | 2:E:369:GLN:OE1   | 2.19                     | 0.43              |
| 2:E:771:TYR:HD2   | 2:E:1212:THR:HG22 | 1.82                     | 0.43              |
| 2:H:552:ILE:HA    | 2:H:555:VAL:HG22  | 2.01                     | 0.43              |
| 2:F:1180:TYR:O    | 2:F:1183:VAL:HG12 | 2.19                     | 0.43              |
| 2:E:1460:LYS:O    | 2:E:1464:LYS:HG2  | 2.19                     | 0.43              |
| 2:H:368:LEU:O     | 2:H:371:THR:HG22  | 2.19                     | 0.43              |
| 2:H:771:TYR:HD1   | 2:H:851:PHE:HD2   | 1.66                     | 0.43              |
| 2:F:521:ARG:O     | 2:F:524:THR:OG1   | 2.36                     | 0.43              |
| 2:F:685:TYR:O     | 2:F:733:VAL:N     | 2.52                     | 0.43              |
| 1:C:158:MET:O     | 1:C:162:ILE:HG12  | 2.19                     | 0.42              |
| 1:D:108:GLU:OE1   | 1:D:108:GLU:N     | 2.52                     | 0.42              |
| 2:E:435:CYS:N     | 2:E:436:PRO:HD2   | 2.33                     | 0.42              |
| 2:E:1180:TYR:O    | 2:E:1183:VAL:HG12 | 2.19                     | 0.42              |
| 2:H:1455:GLU:OE1  | 2:H:1460:LYS:HB3  | 2.18                     | 0.42              |
| 2:G:714:GLN:HE22  | 2:G:1514:ALA:HB3  | 1.84                     | 0.42              |
| 2:G:890:LEU:O     | 2:G:893:LEU:HG    | 2.19                     | 0.42              |
| 2:G:1440:ASP:HB3  | 2:G:1442:GLU:O    | 2.19                     | 0.42              |
| 2:F:141:VAL:O     | 2:F:144:THR:OG1   | 2.32                     | 0.42              |
| 2:F:395:ILE:HG21  | 2:F:421:VAL:HG12  | 2.00                     | 0.42              |
| 2:F:721:SER:HB3   | 2:F:730:MET:HE1   | 2.00                     | 0.42              |
| 1:A:200:LEU:HD22  | 1:A:304:TYR:CE2   | 2.54                     | 0.42              |
| 1:A:242:ASN:OD1   | 1:A:243:GLY:N     | 2.52                     | 0.42              |
| 1:C:122:LEU:O     | 1:C:126:GLU:HG3   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:200:LEU:HD22 | 1:B:304:TYR:CE2   | 2.54                     | 0.42              |
| 2:H:1154:ALA:O   | 2:H:1157:SER:OG   | 2.26                     | 0.42              |
| 2:G:309:ALA:HB1  | 2:G:369:GLN:OE1   | 2.19                     | 0.42              |
| 2:F:127:ILE:HG23 | 2:F:128:GLU:N     | 2.33                     | 0.42              |
| 2:F:1440:ASP:HB3 | 2:F:1442:GLU:O    | 2.19                     | 0.42              |
| 1:B:122:LEU:O    | 1:B:126:GLU:HG3   | 2.19                     | 0.42              |
| 2:E:395:ILE:HG21 | 2:E:421:VAL:HG12  | 2.01                     | 0.42              |
| 2:G:368:LEU:O    | 2:G:371:THR:HG22  | 2.19                     | 0.42              |
| 2:G:552:ILE:HA   | 2:G:555:VAL:HG22  | 2.01                     | 0.42              |
| 2:F:368:LEU:O    | 2:F:371:THR:HG22  | 2.19                     | 0.42              |
| 2:F:714:GLN:HE22 | 2:F:1514:ALA:HB3  | 1.84                     | 0.42              |
| 2:F:1438:ASN:OD1 | 2:F:1474:ILE:HD12 | 2.19                     | 0.42              |
| 1:A:158:MET:O    | 1:A:162:ILE:HG12  | 2.19                     | 0.42              |
| 2:H:107:TYR:CD2  | 2:H:1165:VAL:HG21 | 2.55                     | 0.42              |
| 2:H:685:TYR:O    | 2:H:733:VAL:N     | 2.52                     | 0.42              |
| 2:H:1348:ASN:O   | 2:H:1350:SER:N    | 2.49                     | 0.42              |
| 2:G:435:CYS:N    | 2:G:436:PRO:HD2   | 2.33                     | 0.42              |
| 2:G:685:TYR:O    | 2:G:733:VAL:N     | 2.52                     | 0.42              |
| 2:F:552:ILE:HA   | 2:F:555:VAL:HG22  | 2.01                     | 0.42              |
| 2:F:1376:ILE:HB  | 2:F:1535:ILE:HD13 | 2.00                     | 0.42              |
| 1:C:36:VAL:HB    | 1:C:303:SER:HB3   | 2.01                     | 0.42              |
| 2:E:685:TYR:O    | 2:E:733:VAL:N     | 2.52                     | 0.42              |
| 2:E:1245:ARG:NH2 | 2:E:1248:GLU:OE1  | 2.42                     | 0.42              |
| 2:E:1438:ASN:OD1 | 2:E:1474:ILE:HD12 | 2.19                     | 0.42              |
| 2:H:1142:LEU:HB3 | 2:H:1300:ASN:HB3  | 2.01                     | 0.42              |
| 2:H:1162:VAL:O   | 2:H:1165:VAL:HG22 | 2.20                     | 0.42              |
| 2:H:1440:ASP:HB3 | 2:H:1442:GLU:O    | 2.19                     | 0.42              |
| 2:G:395:ILE:HG21 | 2:G:421:VAL:HG12  | 2.01                     | 0.42              |
| 2:G:1438:ASN:OD1 | 2:G:1474:ILE:HD12 | 2.19                     | 0.42              |
| 1:C:233:LEU:HD21 | 1:B:326:TYR:CE1   | 2.54                     | 0.42              |
| 1:B:158:MET:O    | 1:B:162:ILE:HG12  | 2.19                     | 0.42              |
| 2:E:890:LEU:O    | 2:E:893:LEU:HG    | 2.19                     | 0.42              |
| 2:E:1350:SER:HA  | 2:E:1362:LYS:HA   | 2.02                     | 0.42              |
| 2:H:1350:SER:HA  | 2:H:1362:LYS:HA   | 2.02                     | 0.42              |
| 2:G:1130:THR:O   | 2:G:1134:HIS:HB2  | 2.19                     | 0.42              |
| 2:E:1440:ASP:HB3 | 2:E:1442:GLU:O    | 2.19                     | 0.42              |
| 2:G:314:PHE:HZ   | 2:G:448:GLY:HA2   | 1.83                     | 0.42              |
| 2:G:1162:VAL:O   | 2:G:1165:VAL:HG22 | 2.20                     | 0.42              |
| 2:F:44:PHE:HB2   | 2:F:45:PRO:HD3    | 2.02                     | 0.42              |
| 1:A:180:THR:OG1  | 1:A:205:LEU:HB2   | 2.20                     | 0.42              |
| 1:A:263:ALA:HA   | 1:A:268:TYR:CD1   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:36:VAL:HB     | 1:B:303:SER:HB3   | 2.01                     | 0.42              |
| 2:E:317:PRO:HA    | 2:E:320:ILE:HD12  | 2.02                     | 0.42              |
| 2:E:770:ALA:HA    | 2:E:1216:PHE:CE1  | 2.50                     | 0.42              |
| 2:H:44:PHE:HB2    | 2:H:45:PRO:HD3    | 2.02                     | 0.42              |
| 2:H:716:GLY:N     | 3:H:2004:ATP:O2G  | 2.34                     | 0.42              |
| 2:G:317:PRO:HA    | 2:G:320:ILE:HD12  | 2.02                     | 0.42              |
| 2:G:1350:SER:HA   | 2:G:1362:LYS:HA   | 2.02                     | 0.42              |
| 2:F:890:LEU:O     | 2:F:893:LEU:HG    | 2.19                     | 0.42              |
| 1:C:233:LEU:HD11  | 1:B:326:TYR:CG    | 2.55                     | 0.42              |
| 1:D:95:PHE:HE2    | 2:H:27:PHE:CB     | 2.32                     | 0.42              |
| 2:E:44:PHE:HB2    | 2:E:45:PRO:HD3    | 2.02                     | 0.42              |
| 2:E:368:LEU:O     | 2:E:371:THR:HG22  | 2.19                     | 0.42              |
| 2:H:721:SER:HB3   | 2:H:730:MET:HE1   | 2.00                     | 0.42              |
| 2:G:148:ILE:O     | 2:G:151:THR:OG1   | 2.34                     | 0.42              |
| 2:G:878:ASP:OD2   | 2:G:881:ARG:HB2   | 2.20                     | 0.42              |
| 2:G:1251:MET:HB2  | 2:G:1295:ASN:HD21 | 1.84                     | 0.42              |
| 2:F:39:LEU:HA     | 2:F:42:ILE:HG22   | 2.01                     | 0.42              |
| 1:C:34:ARG:HH21   | 1:C:303:SER:HG    | 1.62                     | 0.42              |
| 1:C:180:THR:OG1   | 1:C:205:LEU:HB2   | 2.20                     | 0.42              |
| 1:B:108:GLU:N     | 1:B:108:GLU:OE1   | 2.52                     | 0.42              |
| 2:E:714:GLN:HE22  | 2:E:1514:ALA:HB3  | 1.84                     | 0.42              |
| 2:H:22:LEU:HB3    | 2:H:156:LYS:HE3   | 2.02                     | 0.42              |
| 2:H:1348:ASN:O    | 2:H:1400:GLY:HA3  | 2.20                     | 0.42              |
| 2:H:1488:LEU:HD13 | 2:H:1488:LEU:HA   | 1.89                     | 0.42              |
| 2:G:107:TYR:CD2   | 2:G:1165:VAL:HG21 | 2.55                     | 0.42              |
| 2:G:553:ALA:O     | 2:G:557:ILE:HG12  | 2.20                     | 0.42              |
| 2:G:1142:LEU:HB3  | 2:G:1300:ASN:HB3  | 2.01                     | 0.42              |
| 2:F:553:ALA:O     | 2:F:557:ILE:HG12  | 2.20                     | 0.42              |
| 1:A:136:ARG:NH1   | 1:B:137:MET:SD    | 2.93                     | 0.41              |
| 1:A:229:GLU:HB3   | 1:D:314:ARG:CZ    | 2.50                     | 0.41              |
| 1:B:180:THR:OG1   | 1:B:205:LEU:HB2   | 2.20                     | 0.41              |
| 2:E:716:GLY:N     | 3:E:2004:ATP:O2G  | 2.34                     | 0.41              |
| 2:E:769:VAL:HG13  | 2:E:849:VAL:O     | 2.20                     | 0.41              |
| 2:E:1163:PHE:CE2  | 2:E:1167:LEU:HB2  | 2.55                     | 0.41              |
| 2:H:317:PRO:HA    | 2:H:320:ILE:HD12  | 2.02                     | 0.41              |
| 2:H:714:GLN:HE22  | 2:H:1514:ALA:HB3  | 1.84                     | 0.41              |
| 2:G:44:PHE:HB2    | 2:G:45:PRO:HD3    | 2.02                     | 0.41              |
| 2:G:1482:SER:HG   | 3:G:2004:ATP:PB   | 2.43                     | 0.41              |
| 2:F:317:PRO:HA    | 2:F:320:ILE:HD12  | 2.02                     | 0.41              |
| 2:F:771:TYR:HD1   | 2:F:851:PHE:HD2   | 1.66                     | 0.41              |
| 2:F:1162:VAL:O    | 2:F:1165:VAL:HG22 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1347:GLN:HE21 | 2:F:1401:HIS:CE1  | 2.38                     | 0.41              |
| 1:B:263:ALA:HA    | 1:B:268:TYR:CD1   | 2.55                     | 0.41              |
| 1:D:36:VAL:HB     | 1:D:303:SER:HB3   | 2.01                     | 0.41              |
| 1:D:263:ALA:HA    | 1:D:268:TYR:CD1   | 2.55                     | 0.41              |
| 2:E:1004:LEU:HB2  | 2:E:1012:LEU:HD21 | 2.03                     | 0.41              |
| 2:H:396:TYR:CG    | 2:H:1226:LEU:HD13 | 2.55                     | 0.41              |
| 2:H:1438:ASN:OD1  | 2:H:1474:ILE:HD12 | 2.19                     | 0.41              |
| 1:D:180:THR:OG1   | 1:D:205:LEU:HB2   | 2.20                     | 0.41              |
| 2:E:22:LEU:HB3    | 2:E:156:LYS:HE3   | 2.02                     | 0.41              |
| 2:E:107:TYR:CD2   | 2:E:1165:VAL:HG21 | 2.55                     | 0.41              |
| 2:E:1142:LEU:HB3  | 2:E:1300:ASN:HB3  | 2.02                     | 0.41              |
| 2:E:1348:ASN:O    | 2:E:1400:GLY:HA3  | 2.20                     | 0.41              |
| 2:H:314:PHE:HZ    | 2:H:448:GLY:HA2   | 1.83                     | 0.41              |
| 2:H:1568:ARG:HH21 | 2:H:1571:SER:HA   | 1.85                     | 0.41              |
| 2:G:1403:ILE:HD13 | 2:G:1408:ASP:HA   | 2.02                     | 0.41              |
| 2:F:22:LEU:HB3    | 2:F:156:LYS:HE3   | 2.02                     | 0.41              |
| 2:F:107:TYR:CD2   | 2:F:1165:VAL:HG21 | 2.55                     | 0.41              |
| 2:F:878:ASP:OD2   | 2:F:881:ARG:HB2   | 2.20                     | 0.41              |
| 2:F:1403:ILE:HD13 | 2:F:1408:ASP:HA   | 2.02                     | 0.41              |
| 1:A:233:LEU:HD11  | 1:D:326:TYR:CG    | 2.56                     | 0.41              |
| 1:C:164:LEU:HD11  | 1:D:164:LEU:HD13  | 2.02                     | 0.41              |
| 1:C:263:ALA:HA    | 1:C:268:TYR:CD1   | 2.55                     | 0.41              |
| 1:C:272:PRO:C     | 1:C:274:ASP:H     | 2.29                     | 0.41              |
| 1:D:158:MET:O     | 1:D:162:ILE:HG12  | 2.19                     | 0.41              |
| 1:D:273:SER:HG    | 2:H:1398:PHE:HE2  | 1.58                     | 0.41              |
| 2:H:769:VAL:HG13  | 2:H:849:VAL:O     | 2.20                     | 0.41              |
| 2:H:878:ASP:OD2   | 2:H:881:ARG:HB2   | 2.20                     | 0.41              |
| 2:H:1251:MET:HB2  | 2:H:1295:ASN:HD21 | 1.84                     | 0.41              |
| 2:G:22:LEU:HB3    | 2:G:156:LYS:HE3   | 2.02                     | 0.41              |
| 2:F:1142:LEU:HB3  | 2:F:1300:ASN:HB3  | 2.02                     | 0.41              |
| 2:F:1251:MET:HB2  | 2:F:1295:ASN:HD21 | 1.84                     | 0.41              |
| 2:F:1350:SER:HA   | 2:F:1362:LYS:HA   | 2.02                     | 0.41              |
| 2:E:437:ASN:ND2   | 2:E:592:LEU:HD23  | 2.29                     | 0.41              |
| 2:E:553:ALA:O     | 2:E:557:ILE:HG12  | 2.20                     | 0.41              |
| 2:E:878:ASP:OD2   | 2:E:881:ARG:HB2   | 2.20                     | 0.41              |
| 2:E:1023:HIS:CE1  | 2:E:1144:ARG:HA   | 2.56                     | 0.41              |
| 2:H:72:ASN:HA     | 2:H:75:TRP:HD1    | 1.85                     | 0.41              |
| 2:H:550:ILE:N     | 2:H:551:PRO:HD2   | 2.36                     | 0.41              |
| 2:H:1004:LEU:HB2  | 2:H:1012:LEU:HD21 | 2.03                     | 0.41              |
| 2:H:1346:ILE:HG22 | 2:H:1402:ILE:HG13 | 2.02                     | 0.41              |
| 2:G:1347:GLN:HE21 | 2:G:1401:HIS:CE1  | 2.38                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:6:CYS:H       | 2:F:16:ARG:HH11   | 1.69                     | 0.41              |
| 2:F:84:VAL:HG11   | 2:F:174:LEU:HD12  | 2.03                     | 0.41              |
| 2:F:805:CYS:O     | 2:F:836:ARG:HD2   | 2.20                     | 0.41              |
| 2:F:1163:PHE:CE2  | 2:F:1167:LEU:HB2  | 2.56                     | 0.41              |
| 2:F:1568:ARG:HH21 | 2:F:1571:SER:HA   | 1.85                     | 0.41              |
| 1:C:218:GLN:NE2   | 1:C:235:GLN:HB3   | 2.35                     | 0.41              |
| 2:E:1162:VAL:O    | 2:E:1165:VAL:HG22 | 2.20                     | 0.41              |
| 2:E:1251:MET:HB2  | 2:E:1295:ASN:HD21 | 1.84                     | 0.41              |
| 2:E:1346:ILE:HG22 | 2:E:1402:ILE:HG13 | 2.02                     | 0.41              |
| 2:H:1163:PHE:CE2  | 2:H:1167:LEU:HB2  | 2.56                     | 0.41              |
| 2:F:716:GLY:N     | 3:F:2004:ATP:O2G  | 2.34                     | 0.41              |
| 2:F:1346:ILE:HG22 | 2:F:1402:ILE:HG13 | 2.02                     | 0.41              |
| 1:C:314:ARG:CZ    | 1:D:229:GLU:HB3   | 2.51                     | 0.41              |
| 2:E:6:CYS:H       | 2:E:16:ARG:HH11   | 1.68                     | 0.41              |
| 2:H:84:VAL:HG11   | 2:H:174:LEU:HD12  | 2.03                     | 0.41              |
| 2:H:320:ILE:HG23  | 2:H:1284:LEU:HD11 | 2.03                     | 0.41              |
| 2:H:428:LEU:HD23  | 2:H:428:LEU:HA    | 1.91                     | 0.41              |
| 2:H:553:ALA:O     | 2:H:557:ILE:HG12  | 2.20                     | 0.41              |
| 2:G:396:TYR:CG    | 2:G:1226:LEU:HD13 | 2.55                     | 0.41              |
| 2:G:1023:HIS:CE1  | 2:G:1144:ARG:HA   | 2.56                     | 0.41              |
| 2:G:1348:ASN:O    | 2:G:1400:GLY:HA3  | 2.20                     | 0.41              |
| 2:F:1255:GLY:O    | 2:F:1259:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:36:VAL:HB     | 1:A:303:SER:HB3   | 2.01                     | 0.41              |
| 2:E:72:ASN:HA     | 2:E:75:TRP:HD1    | 1.85                     | 0.41              |
| 2:E:709:THR:HA    | 2:E:898:TRP:O     | 2.21                     | 0.41              |
| 2:E:1267:ILE:O    | 2:E:1268:SER:C    | 2.64                     | 0.41              |
| 2:H:147:PHE:O     | 2:H:151:THR:HG23  | 2.21                     | 0.41              |
| 2:H:1255:GLY:O    | 2:H:1259:VAL:HG23 | 2.21                     | 0.41              |
| 2:G:84:VAL:HG11   | 2:G:174:LEU:HD12  | 2.03                     | 0.41              |
| 2:G:769:VAL:HG13  | 2:G:849:VAL:O     | 2.21                     | 0.41              |
| 2:G:1568:ARG:HH21 | 2:G:1571:SER:HA   | 1.85                     | 0.41              |
| 2:F:302:SER:OG    | 2:F:376:SER:O     | 2.31                     | 0.41              |
| 2:F:1023:HIS:CE1  | 2:F:1144:ARG:HA   | 2.56                     | 0.41              |
| 1:A:272:PRO:C     | 1:A:274:ASP:H     | 2.29                     | 0.41              |
| 1:C:95:PHE:HE2    | 2:G:27:PHE:CB     | 2.34                     | 0.41              |
| 1:C:242:ASN:OD1   | 1:C:243:GLY:N     | 2.52                     | 0.41              |
| 1:C:314:ARG:HD2   | 1:D:229:GLU:OE1   | 2.21                     | 0.41              |
| 1:B:74:ILE:HD13   | 2:F:49:ILE:HG22   | 2.03                     | 0.41              |
| 1:B:272:PRO:C     | 1:B:274:ASP:H     | 2.29                     | 0.41              |
| 1:B:335:ASN:HD22  | 1:B:336:THR:H     | 1.69                     | 0.41              |
| 2:E:396:TYR:CG    | 2:E:1226:LEU:HD13 | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:550:ILE:N     | 2:E:551:PRO:HD2   | 2.36                     | 0.41              |
| 2:E:709:THR:HB    | 2:E:898:TRP:HB3   | 2.03                     | 0.41              |
| 2:E:1255:GLY:O    | 2:E:1259:VAL:HG23 | 2.21                     | 0.41              |
| 2:G:72:ASN:HA     | 2:G:75:TRP:HD1    | 1.85                     | 0.41              |
| 2:G:147:PHE:O     | 2:G:151:THR:HG23  | 2.21                     | 0.41              |
| 2:G:777:TRP:CZ3   | 2:G:1209:GLY:HA3  | 2.56                     | 0.41              |
| 2:G:1255:GLY:O    | 2:G:1259:VAL:HG23 | 2.21                     | 0.41              |
| 2:G:1267:ILE:O    | 2:G:1268:SER:C    | 2.64                     | 0.41              |
| 2:F:72:ASN:HA     | 2:F:75:TRP:HD1    | 1.85                     | 0.41              |
| 2:F:314:PHE:CE2   | 2:F:447:VAL:HG12  | 2.56                     | 0.41              |
| 2:F:320:ILE:HG23  | 2:F:1284:LEU:HD11 | 2.03                     | 0.41              |
| 2:F:396:TYR:CG    | 2:F:1226:LEU:HD13 | 2.55                     | 0.41              |
| 2:F:550:ILE:N     | 2:F:551:PRO:HD2   | 2.35                     | 0.41              |
| 2:F:889:LYS:HZ2   | 2:F:892:TYR:HE2   | 1.69                     | 0.41              |
| 1:A:184:SER:O     | 1:A:304:TYR:OH    | 2.32                     | 0.41              |
| 1:D:242:ASN:OD1   | 1:D:243:GLY:N     | 2.52                     | 0.41              |
| 2:E:1347:GLN:HE21 | 2:E:1401:HIS:CE1  | 2.38                     | 0.41              |
| 2:E:1568:ARG:HH21 | 2:E:1571:SER:HA   | 1.85                     | 0.41              |
| 2:G:679:VAL:HA    | 2:G:738:PHE:O     | 2.21                     | 0.41              |
| 2:G:709:THR:HA    | 2:G:898:TRP:O     | 2.21                     | 0.41              |
| 2:G:1131:ILE:HA   | 2:G:1135:ILE:CD1  | 2.51                     | 0.41              |
| 2:E:84:VAL:HG11   | 2:E:174:LEU:HD12  | 2.03                     | 0.40              |
| 2:E:805:CYS:O     | 2:E:836:ARG:HD2   | 2.20                     | 0.40              |
| 2:G:805:CYS:O     | 2:G:836:ARG:HD2   | 2.20                     | 0.40              |
| 2:G:1346:ILE:HG22 | 2:G:1402:ILE:HG13 | 2.02                     | 0.40              |
| 2:F:709:THR:HA    | 2:F:898:TRP:O     | 2.21                     | 0.40              |
| 2:F:1004:LEU:HB2  | 2:F:1012:LEU:HD21 | 2.03                     | 0.40              |
| 2:H:679:VAL:HA    | 2:H:738:PHE:O     | 2.21                     | 0.40              |
| 2:H:709:THR:HA    | 2:H:898:TRP:O     | 2.21                     | 0.40              |
| 2:G:36:HIS:HD2    | 2:G:142:TYR:CE1   | 2.40                     | 0.40              |
| 2:G:374:GLN:NE2   | 2:G:1245:ARG:HE   | 2.20                     | 0.40              |
| 2:G:808:GLN:HB2   | 2:G:809:PRO:HD3   | 2.03                     | 0.40              |
| 2:F:777:TRP:CZ3   | 2:F:1209:GLY:HA3  | 2.56                     | 0.40              |
| 2:F:1348:ASN:O    | 2:F:1400:GLY:HA3  | 2.20                     | 0.40              |
| 1:A:146:ILE:HG12  | 1:D:122:LEU:HD21  | 2.02                     | 0.40              |
| 1:D:218:GLN:NE2   | 1:D:235:GLN:HB3   | 2.35                     | 0.40              |
| 1:D:335:ASN:HD22  | 1:D:336:THR:H     | 1.69                     | 0.40              |
| 2:E:147:PHE:O     | 2:E:151:THR:HG23  | 2.21                     | 0.40              |
| 2:H:805:CYS:O     | 2:H:836:ARG:HD2   | 2.20                     | 0.40              |
| 2:H:1131:ILE:HA   | 2:H:1135:ILE:CD1  | 2.51                     | 0.40              |
| 2:H:1347:GLN:HE21 | 2:H:1401:HIS:CE1  | 2.38                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:320:ILE:HG23  | 2:G:1284:LEU:HD11 | 2.03                     | 0.40              |
| 2:G:1004:LEU:HB2  | 2:G:1012:LEU:HD21 | 2.03                     | 0.40              |
| 2:G:1065:MET:O    | 2:G:1068:THR:OG1  | 2.33                     | 0.40              |
| 2:G:1292:ASN:HD22 | 2:G:1292:ASN:C    | 2.29                     | 0.40              |
| 2:F:370:ARG:HB3   | 2:F:1252:GLU:HG2  | 2.04                     | 0.40              |
| 2:F:1505:ASP:HA   | 2:F:1535:ILE:HB   | 2.03                     | 0.40              |
| 1:D:272:PRO:C     | 1:D:274:ASP:H     | 2.29                     | 0.40              |
| 2:E:370:ARG:HB3   | 2:E:1252:GLU:HG2  | 2.04                     | 0.40              |
| 2:H:717:CYS:O     | 2:H:905:GLY:N     | 2.54                     | 0.40              |
| 2:H:1031:TYR:CE2  | 2:H:1035:LYS:HD2  | 2.57                     | 0.40              |
| 2:G:1163:PHE:CE2  | 2:G:1167:LEU:HB2  | 2.55                     | 0.40              |
| 2:F:717:CYS:O     | 2:F:905:GLY:N     | 2.54                     | 0.40              |
| 1:A:326:TYR:CZ    | 1:B:233:LEU:HD21  | 2.57                     | 0.40              |
| 1:C:136:ARG:HH12  | 1:D:137:MET:CG    | 2.34                     | 0.40              |
| 1:C:229:GLU:OE1   | 1:B:314:ARG:HD2   | 2.22                     | 0.40              |
| 2:E:808:GLN:HB2   | 2:E:809:PRO:HD3   | 2.03                     | 0.40              |
| 2:H:709:THR:HB    | 2:H:898:TRP:HB3   | 2.03                     | 0.40              |
| 2:H:808:GLN:HB2   | 2:H:809:PRO:HD3   | 2.03                     | 0.40              |
| 2:G:550:ILE:N     | 2:G:551:PRO:HD2   | 2.35                     | 0.40              |
| 2:G:1031:TYR:CE2  | 2:G:1035:LYS:HD2  | 2.57                     | 0.40              |
| 2:G:1505:ASP:HA   | 2:G:1535:ILE:HB   | 2.03                     | 0.40              |
| 2:F:709:THR:HB    | 2:F:898:TRP:HB3   | 2.03                     | 0.40              |
| 2:F:769:VAL:HG13  | 2:F:849:VAL:O     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 326/406 (80%) | 301 (92%) | 25 (8%) | 0        | 100         | 100 |
| 1   | B     | 326/406 (80%) | 302 (93%) | 24 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | C     | 326/406 (80%)   | 303 (93%)  | 23 (7%)  | 0        | 100         | 100 |
| 1   | D     | 326/406 (80%)   | 303 (93%)  | 23 (7%)  | 0        | 100         | 100 |
| 2   | E     | 1270/1581 (80%) | 1175 (92%) | 95 (8%)  | 0        | 100         | 100 |
| 2   | F     | 1270/1581 (80%) | 1175 (92%) | 95 (8%)  | 0        | 100         | 100 |
| 2   | G     | 1270/1581 (80%) | 1175 (92%) | 95 (8%)  | 0        | 100         | 100 |
| 2   | H     | 1270/1581 (80%) | 1175 (92%) | 95 (8%)  | 0        | 100         | 100 |
| All | All   | 6384/7948 (80%) | 5909 (93%) | 475 (7%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 264/348 (76%)   | 264 (100%)  | 0        | 100         | 100 |
| 1   | B     | 264/348 (76%)   | 264 (100%)  | 0        | 100         | 100 |
| 1   | C     | 264/348 (76%)   | 264 (100%)  | 0        | 100         | 100 |
| 1   | D     | 264/348 (76%)   | 264 (100%)  | 0        | 100         | 100 |
| 2   | E     | 987/1368 (72%)  | 983 (100%)  | 4 (0%)   | 84          | 83  |
| 2   | F     | 987/1368 (72%)  | 983 (100%)  | 4 (0%)   | 84          | 83  |
| 2   | G     | 987/1368 (72%)  | 983 (100%)  | 4 (0%)   | 84          | 83  |
| 2   | H     | 987/1368 (72%)  | 983 (100%)  | 4 (0%)   | 84          | 83  |
| All | All   | 5004/6864 (73%) | 4988 (100%) | 16 (0%)  | 84          | 85  |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1142 | LEU  |
| 2   | E     | 1271 | LEU  |
| 2   | E     | 1511 | ILE  |
| 2   | E     | 1513 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | H     | 1142 | LEU  |
| 2   | H     | 1271 | LEU  |
| 2   | H     | 1511 | ILE  |
| 2   | H     | 1513 | MET  |
| 2   | G     | 1142 | LEU  |
| 2   | G     | 1271 | LEU  |
| 2   | G     | 1511 | ILE  |
| 2   | G     | 1513 | MET  |
| 2   | F     | 1142 | LEU  |
| 2   | F     | 1271 | LEU  |
| 2   | F     | 1511 | ILE  |
| 2   | F     | 1513 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | HIS  |
| 1   | A     | 115 | HIS  |
| 1   | A     | 186 | HIS  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 235 | GLN  |
| 1   | A     | 277 | HIS  |
| 1   | A     | 335 | ASN  |
| 1   | C     | 70  | HIS  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 186 | HIS  |
| 1   | C     | 193 | HIS  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 277 | HIS  |
| 1   | C     | 335 | ASN  |
| 1   | B     | 115 | HIS  |
| 1   | B     | 186 | HIS  |
| 1   | B     | 218 | GLN  |
| 1   | B     | 235 | GLN  |
| 1   | B     | 277 | HIS  |
| 1   | B     | 335 | ASN  |
| 1   | D     | 115 | HIS  |
| 1   | D     | 186 | HIS  |
| 1   | D     | 218 | GLN  |
| 1   | D     | 277 | HIS  |
| 1   | D     | 335 | ASN  |
| 2   | E     | 36  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 102  | HIS  |
| 2   | E     | 126  | ASN  |
| 2   | E     | 188  | ASN  |
| 2   | E     | 416  | GLN  |
| 2   | E     | 419  | ASN  |
| 2   | E     | 427  | GLN  |
| 2   | E     | 437  | ASN  |
| 2   | E     | 474  | GLN  |
| 2   | E     | 498  | GLN  |
| 2   | E     | 500  | ASN  |
| 2   | E     | 608  | GLN  |
| 2   | E     | 680  | GLN  |
| 2   | E     | 714  | GLN  |
| 2   | E     | 780  | ASN  |
| 2   | E     | 816  | HIS  |
| 2   | E     | 821  | GLN  |
| 2   | E     | 835  | GLN  |
| 2   | E     | 1129 | ASN  |
| 2   | E     | 1133 | GLN  |
| 2   | E     | 1202 | HIS  |
| 2   | E     | 1244 | ASN  |
| 2   | E     | 1272 | HIS  |
| 2   | E     | 1347 | GLN  |
| 2   | E     | 1363 | HIS  |
| 2   | E     | 1485 | GLN  |
| 2   | H     | 36   | HIS  |
| 2   | H     | 102  | HIS  |
| 2   | H     | 125  | HIS  |
| 2   | H     | 126  | ASN  |
| 2   | H     | 188  | ASN  |
| 2   | H     | 416  | GLN  |
| 2   | H     | 419  | ASN  |
| 2   | H     | 427  | GLN  |
| 2   | H     | 437  | ASN  |
| 2   | H     | 474  | GLN  |
| 2   | H     | 498  | GLN  |
| 2   | H     | 500  | ASN  |
| 2   | H     | 608  | GLN  |
| 2   | H     | 680  | GLN  |
| 2   | H     | 714  | GLN  |
| 2   | H     | 780  | ASN  |
| 2   | H     | 821  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | H     | 835  | GLN  |
| 2   | H     | 1129 | ASN  |
| 2   | H     | 1133 | GLN  |
| 2   | H     | 1202 | HIS  |
| 2   | H     | 1244 | ASN  |
| 2   | H     | 1272 | HIS  |
| 2   | H     | 1292 | ASN  |
| 2   | H     | 1347 | GLN  |
| 2   | H     | 1363 | HIS  |
| 2   | H     | 1485 | GLN  |
| 2   | G     | 36   | HIS  |
| 2   | G     | 102  | HIS  |
| 2   | G     | 126  | ASN  |
| 2   | G     | 188  | ASN  |
| 2   | G     | 416  | GLN  |
| 2   | G     | 419  | ASN  |
| 2   | G     | 427  | GLN  |
| 2   | G     | 437  | ASN  |
| 2   | G     | 474  | GLN  |
| 2   | G     | 498  | GLN  |
| 2   | G     | 500  | ASN  |
| 2   | G     | 608  | GLN  |
| 2   | G     | 680  | GLN  |
| 2   | G     | 714  | GLN  |
| 2   | G     | 780  | ASN  |
| 2   | G     | 816  | HIS  |
| 2   | G     | 821  | GLN  |
| 2   | G     | 835  | GLN  |
| 2   | G     | 1129 | ASN  |
| 2   | G     | 1133 | GLN  |
| 2   | G     | 1202 | HIS  |
| 2   | G     | 1244 | ASN  |
| 2   | G     | 1272 | HIS  |
| 2   | G     | 1347 | GLN  |
| 2   | G     | 1363 | HIS  |
| 2   | F     | 36   | HIS  |
| 2   | F     | 102  | HIS  |
| 2   | F     | 126  | ASN  |
| 2   | F     | 188  | ASN  |
| 2   | F     | 416  | GLN  |
| 2   | F     | 419  | ASN  |
| 2   | F     | 427  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | F     | 437  | ASN  |
| 2   | F     | 474  | GLN  |
| 2   | F     | 498  | GLN  |
| 2   | F     | 500  | ASN  |
| 2   | F     | 608  | GLN  |
| 2   | F     | 680  | GLN  |
| 2   | F     | 714  | GLN  |
| 2   | F     | 780  | ASN  |
| 2   | F     | 821  | GLN  |
| 2   | F     | 835  | GLN  |
| 2   | F     | 1129 | ASN  |
| 2   | F     | 1133 | GLN  |
| 2   | F     | 1202 | HIS  |
| 2   | F     | 1244 | ASN  |
| 2   | F     | 1272 | HIS  |
| 2   | F     | 1347 | GLN  |
| 2   | F     | 1363 | HIS  |

### 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](#)

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ATP  | H     | 2004 | 6    | 32,33,33     | 1.30 | 5 (15%)  | 48,52,52    | 1.77 | 12 (25%) |
| 3   | ATP  | D     | 501  | -    | 32,33,33     | 1.27 | 5 (15%)  | 48,52,52    | 1.79 | 12 (25%) |
| 5   | ADP  | G     | 2001 | 6    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.79 | 8 (18%)  |
| 5   | ADP  | E     | 2001 | 6    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.78 | 9 (20%)  |
| 3   | ATP  | E     | 2004 | 6    | 32,33,33     | 1.31 | 5 (15%)  | 48,52,52    | 1.77 | 12 (25%) |
| 5   | ADP  | F     | 2001 | 6    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.79 | 9 (20%)  |
| 3   | ATP  | F     | 2004 | 6    | 32,33,33     | 1.31 | 5 (15%)  | 48,52,52    | 1.78 | 11 (22%) |
| 5   | ADP  | H     | 2001 | 6    | 28,29,29     | 1.37 | 5 (17%)  | 43,45,45    | 1.78 | 9 (20%)  |
| 3   | ATP  | A     | 501  | -    | 32,33,33     | 1.29 | 5 (15%)  | 48,52,52    | 1.78 | 9 (18%)  |
| 3   | ATP  | G     | 2004 | 6    | 32,33,33     | 1.30 | 5 (15%)  | 48,52,52    | 1.76 | 12 (25%) |
| 3   | ATP  | B     | 501  | -    | 32,33,33     | 1.29 | 5 (15%)  | 48,52,52    | 1.79 | 9 (18%)  |
| 3   | ATP  | C     | 501  | -    | 32,33,33     | 1.28 | 5 (15%)  | 48,52,52    | 1.80 | 9 (18%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | ATP  | H     | 2004 | 6    | -       | 0/22/38/38 | 0/3/3/3 |
| 3   | ATP  | D     | 501  | -    | -       | 3/22/38/38 | 0/3/3/3 |
| 5   | ADP  | G     | 2001 | 6    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | ADP  | E     | 2001 | 6    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ATP  | E     | 2004 | 6    | -       | 0/22/38/38 | 0/3/3/3 |
| 5   | ADP  | F     | 2001 | 6    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ATP  | F     | 2004 | 6    | -       | 0/22/38/38 | 0/3/3/3 |
| 5   | ADP  | H     | 2001 | 6    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ATP  | A     | 501  | -    | -       | 0/22/38/38 | 0/3/3/3 |
| 3   | ATP  | G     | 2004 | 6    | -       | 0/22/38/38 | 0/3/3/3 |
| 3   | ATP  | B     | 501  | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 3   | ATP  | C     | 501  | -    | -       | 2/22/38/38 | 0/3/3/3 |

All (60) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | F     | 2001 | ADP  | C5-C4 | 4.49 | 1.47        | 1.39     |
| 5   | G     | 2001 | ADP  | C5-C4 | 4.47 | 1.47        | 1.39     |
| 3   | F     | 2004 | ATP  | C5-C4 | 4.47 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | E     | 2001 | ADP  | C5-C4 | 4.47  | 1.47        | 1.39     |
| 3   | B     | 501  | ATP  | C5-C4 | 4.45  | 1.47        | 1.39     |
| 3   | E     | 2004 | ATP  | C5-C4 | 4.45  | 1.47        | 1.39     |
| 3   | C     | 501  | ATP  | C5-C4 | 4.42  | 1.47        | 1.39     |
| 5   | H     | 2001 | ADP  | C5-C4 | 4.41  | 1.47        | 1.39     |
| 3   | A     | 501  | ATP  | C5-C4 | 4.39  | 1.46        | 1.39     |
| 3   | H     | 2004 | ATP  | C5-C4 | 4.36  | 1.46        | 1.39     |
| 3   | G     | 2004 | ATP  | C5-C4 | 4.35  | 1.46        | 1.39     |
| 3   | D     | 501  | ATP  | C5-C4 | 4.30  | 1.46        | 1.39     |
| 3   | C     | 501  | ATP  | C5-N7 | -2.58 | 1.34        | 1.39     |
| 5   | F     | 2001 | ADP  | C5-C6 | 2.56  | 1.48        | 1.41     |
| 3   | G     | 2004 | ATP  | C5-C6 | 2.56  | 1.48        | 1.41     |
| 5   | E     | 2001 | ADP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 3   | H     | 2004 | ATP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 5   | G     | 2001 | ADP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 3   | E     | 2004 | ATP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | A     | 501  | ATP  | C5-N7 | -2.53 | 1.34        | 1.39     |
| 5   | H     | 2001 | ADP  | C5-C6 | 2.52  | 1.48        | 1.41     |
| 3   | F     | 2004 | ATP  | C5-C6 | 2.52  | 1.48        | 1.41     |
| 5   | E     | 2001 | ADP  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 3   | B     | 501  | ATP  | C5-N7 | -2.51 | 1.34        | 1.39     |
| 5   | G     | 2001 | ADP  | C5-N7 | -2.51 | 1.34        | 1.39     |
| 3   | B     | 501  | ATP  | C5-C6 | 2.50  | 1.48        | 1.41     |
| 3   | D     | 501  | ATP  | C5-N7 | -2.48 | 1.34        | 1.39     |
| 3   | D     | 501  | ATP  | C5-C6 | 2.47  | 1.47        | 1.41     |
| 5   | H     | 2001 | ADP  | C5-N7 | -2.46 | 1.34        | 1.39     |
| 5   | F     | 2001 | ADP  | C5-N7 | -2.46 | 1.34        | 1.39     |
| 3   | F     | 2004 | ATP  | C5-N7 | -2.46 | 1.34        | 1.39     |
| 3   | E     | 2004 | ATP  | C5-N7 | -2.46 | 1.34        | 1.39     |
| 3   | C     | 501  | ATP  | C5-C6 | 2.45  | 1.47        | 1.41     |
| 3   | A     | 501  | ATP  | C5-C6 | 2.45  | 1.47        | 1.41     |
| 3   | G     | 2004 | ATP  | C5-N7 | -2.45 | 1.34        | 1.39     |
| 3   | H     | 2004 | ATP  | C5-N7 | -2.36 | 1.34        | 1.39     |
| 3   | D     | 501  | ATP  | C8-N7 | 2.28  | 1.36        | 1.31     |
| 3   | D     | 501  | ATP  | C4-N9 | -2.25 | 1.33        | 1.37     |
| 3   | F     | 2004 | ATP  | C4-N9 | -2.25 | 1.33        | 1.37     |
| 5   | G     | 2001 | ADP  | C8-N7 | 2.24  | 1.36        | 1.31     |
| 3   | G     | 2004 | ATP  | C4-N9 | -2.23 | 1.33        | 1.37     |
| 3   | H     | 2004 | ATP  | C4-N9 | -2.23 | 1.33        | 1.37     |
| 3   | B     | 501  | ATP  | C8-N7 | 2.21  | 1.35        | 1.31     |
| 3   | A     | 501  | ATP  | C4-N9 | -2.20 | 1.33        | 1.37     |
| 5   | E     | 2001 | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | H     | 2001 | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 5   | F     | 2001 | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 3   | E     | 2004 | ATP  | C4-N9 | -2.19 | 1.33        | 1.37     |
| 3   | A     | 501  | ATP  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 3   | C     | 501  | ATP  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 3   | B     | 501  | ATP  | C4-N9 | -2.16 | 1.33        | 1.37     |
| 3   | H     | 2004 | ATP  | C8-N7 | 2.15  | 1.35        | 1.31     |
| 3   | G     | 2004 | ATP  | C8-N7 | 2.14  | 1.35        | 1.31     |
| 5   | G     | 2001 | ADP  | C4-N9 | -2.13 | 1.33        | 1.37     |
| 3   | C     | 501  | ATP  | C4-N9 | -2.12 | 1.33        | 1.37     |
| 3   | E     | 2004 | ATP  | C8-N7 | 2.11  | 1.35        | 1.31     |
| 5   | F     | 2001 | ADP  | C4-N9 | -2.10 | 1.33        | 1.37     |
| 3   | F     | 2004 | ATP  | C8-N7 | 2.09  | 1.35        | 1.31     |
| 5   | E     | 2001 | ADP  | C4-N9 | -2.08 | 1.33        | 1.37     |
| 5   | H     | 2001 | ADP  | C4-N9 | -2.07 | 1.33        | 1.37     |

All (121) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | C     | 501  | ATP  | C5-C4-N3 | -5.85 | 118.66      | 126.72   |
| 3   | B     | 501  | ATP  | C5-C4-N3 | -5.79 | 118.74      | 126.72   |
| 3   | A     | 501  | ATP  | C5-C4-N3 | -5.73 | 118.82      | 126.72   |
| 5   | G     | 2001 | ADP  | C5-C4-N3 | -5.64 | 118.95      | 126.72   |
| 3   | F     | 2004 | ATP  | C5-C4-N3 | -5.62 | 118.98      | 126.72   |
| 5   | F     | 2001 | ADP  | C5-C4-N3 | -5.61 | 118.99      | 126.72   |
| 5   | E     | 2001 | ADP  | C5-C4-N3 | -5.61 | 119.00      | 126.72   |
| 5   | H     | 2001 | ADP  | C5-C4-N3 | -5.60 | 119.00      | 126.72   |
| 3   | H     | 2004 | ATP  | C5-C4-N3 | -5.57 | 119.05      | 126.72   |
| 3   | E     | 2004 | ATP  | C5-C4-N3 | -5.56 | 119.06      | 126.72   |
| 3   | D     | 501  | ATP  | C5-C4-N3 | -5.51 | 119.13      | 126.72   |
| 3   | G     | 2004 | ATP  | C5-C4-N3 | -5.50 | 119.14      | 126.72   |
| 3   | C     | 501  | ATP  | N3-C4-N9 | 4.66  | 135.09      | 127.17   |
| 3   | B     | 501  | ATP  | N3-C4-N9 | 4.56  | 134.93      | 127.17   |
| 3   | A     | 501  | ATP  | N3-C4-N9 | 4.53  | 134.87      | 127.17   |
| 3   | E     | 2004 | ATP  | N3-C4-N9 | 4.50  | 134.82      | 127.17   |
| 3   | F     | 2004 | ATP  | N3-C4-N9 | 4.49  | 134.81      | 127.17   |
| 5   | F     | 2001 | ADP  | N3-C4-N9 | 4.48  | 134.79      | 127.17   |
| 5   | E     | 2001 | ADP  | N3-C4-N9 | 4.46  | 134.75      | 127.17   |
| 5   | G     | 2001 | ADP  | N3-C4-N9 | 4.46  | 134.74      | 127.17   |
| 3   | H     | 2004 | ATP  | N3-C4-N9 | 4.44  | 134.72      | 127.17   |
| 3   | G     | 2004 | ATP  | N3-C4-N9 | 4.43  | 134.71      | 127.17   |
| 5   | H     | 2001 | ADP  | N3-C4-N9 | 4.42  | 134.68      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 501  | ATP  | N3-C4-N9 | 4.34  | 134.54      | 127.17   |
| 3   | C     | 501  | ATP  | C2-N3-C4 | 3.67  | 120.80      | 111.83   |
| 3   | B     | 501  | ATP  | C2-N3-C4 | 3.67  | 120.79      | 111.83   |
| 3   | A     | 501  | ATP  | C2-N3-C4 | 3.63  | 120.70      | 111.83   |
| 5   | G     | 2001 | ADP  | C2-N3-C4 | 3.60  | 120.62      | 111.83   |
| 3   | D     | 501  | ATP  | C2-N3-C4 | 3.58  | 120.58      | 111.83   |
| 5   | F     | 2001 | ADP  | C2-N3-C4 | 3.58  | 120.57      | 111.83   |
| 5   | E     | 2001 | ADP  | C2-N3-C4 | 3.57  | 120.55      | 111.83   |
| 5   | H     | 2001 | ADP  | C2-N3-C4 | 3.57  | 120.55      | 111.83   |
| 3   | F     | 2004 | ATP  | C2-N3-C4 | 3.49  | 120.36      | 111.83   |
| 3   | E     | 2004 | ATP  | C2-N3-C4 | 3.46  | 120.28      | 111.83   |
| 3   | F     | 2004 | ATP  | C4-C5-N7 | -3.46 | 106.63      | 110.58   |
| 3   | H     | 2004 | ATP  | C4-C5-N7 | -3.45 | 106.63      | 110.58   |
| 3   | H     | 2004 | ATP  | C2-N3-C4 | 3.43  | 120.22      | 111.83   |
| 3   | G     | 2004 | ATP  | C2-N3-C4 | 3.43  | 120.20      | 111.83   |
| 3   | E     | 2004 | ATP  | C4-C5-N7 | -3.41 | 106.68      | 110.58   |
| 3   | G     | 2004 | ATP  | C4-C5-N7 | -3.38 | 106.71      | 110.58   |
| 3   | B     | 501  | ATP  | C4-C5-N7 | -3.37 | 106.72      | 110.58   |
| 3   | C     | 501  | ATP  | C4-C5-N7 | -3.35 | 106.75      | 110.58   |
| 3   | D     | 501  | ATP  | C4-C5-N7 | -3.34 | 106.76      | 110.58   |
| 5   | H     | 2001 | ADP  | C4-C5-N7 | -3.33 | 106.77      | 110.58   |
| 3   | A     | 501  | ATP  | C4-C5-N7 | -3.32 | 106.79      | 110.58   |
| 5   | E     | 2001 | ADP  | C4-C5-N7 | -3.30 | 106.81      | 110.58   |
| 5   | G     | 2001 | ADP  | C4-C5-N7 | -3.30 | 106.81      | 110.58   |
| 5   | F     | 2001 | ADP  | C4-C5-N7 | -3.29 | 106.82      | 110.58   |
| 3   | D     | 501  | ATP  | N3-C2-N1 | -3.23 | 123.70      | 128.58   |
| 5   | G     | 2001 | ADP  | N3-C2-N1 | -3.18 | 123.77      | 128.58   |
| 3   | A     | 501  | ATP  | N3-C2-N1 | -3.18 | 123.78      | 128.58   |
| 3   | B     | 501  | ATP  | N3-C2-N1 | -3.16 | 123.79      | 128.58   |
| 3   | C     | 501  | ATP  | N3-C2-N1 | -3.16 | 123.80      | 128.58   |
| 5   | E     | 2001 | ADP  | N3-C2-N1 | -3.14 | 123.82      | 128.58   |
| 5   | F     | 2001 | ADP  | N3-C2-N1 | -3.14 | 123.82      | 128.58   |
| 5   | H     | 2001 | ADP  | N3-C2-N1 | -3.14 | 123.84      | 128.58   |
| 3   | F     | 2004 | ATP  | N3-C2-N1 | -3.00 | 124.04      | 128.58   |
| 3   | E     | 2004 | ATP  | N3-C2-N1 | -2.99 | 124.06      | 128.58   |
| 3   | G     | 2004 | ATP  | C4-N9-C8 | 2.98  | 108.87      | 105.74   |
| 3   | H     | 2004 | ATP  | N3-C2-N1 | -2.98 | 124.08      | 128.58   |
| 3   | H     | 2004 | ATP  | C4-N9-C8 | 2.97  | 108.86      | 105.74   |
| 3   | G     | 2004 | ATP  | N3-C2-N1 | -2.97 | 124.09      | 128.58   |
| 3   | E     | 2004 | ATP  | C4-N9-C8 | 2.95  | 108.84      | 105.74   |
| 3   | F     | 2004 | ATP  | C4-N9-C8 | 2.88  | 108.77      | 105.74   |
| 3   | D     | 501  | ATP  | C4-N9-C8 | 2.84  | 108.72      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | C     | 501  | ATP  | C4-N9-C8    | 2.67  | 108.54      | 105.74   |
| 5   | F     | 2001 | ADP  | C4-N9-C8    | 2.66  | 108.53      | 105.74   |
| 3   | B     | 501  | ATP  | C4-N9-C8    | 2.66  | 108.53      | 105.74   |
| 3   | A     | 501  | ATP  | C4-N9-C8    | 2.66  | 108.53      | 105.74   |
| 5   | G     | 2001 | ADP  | C4-N9-C8    | 2.63  | 108.50      | 105.74   |
| 5   | E     | 2001 | ADP  | C4-N9-C8    | 2.62  | 108.49      | 105.74   |
| 5   | H     | 2001 | ADP  | C4-N9-C8    | 2.59  | 108.46      | 105.74   |
| 3   | A     | 501  | ATP  | C3'-C2'-C1' | 2.56  | 106.31      | 101.46   |
| 3   | C     | 501  | ATP  | C3'-C2'-C1' | 2.51  | 106.20      | 101.46   |
| 3   | F     | 2004 | ATP  | C5-N7-C8    | 2.49  | 107.37      | 103.45   |
| 3   | E     | 2004 | ATP  | C5-N7-C8    | 2.48  | 107.35      | 103.45   |
| 3   | B     | 501  | ATP  | C3'-C2'-C1' | 2.48  | 106.15      | 101.46   |
| 3   | H     | 2004 | ATP  | C5-N7-C8    | 2.48  | 107.34      | 103.45   |
| 3   | D     | 501  | ATP  | C3'-C2'-C1' | 2.46  | 106.12      | 101.46   |
| 3   | G     | 2004 | ATP  | C5-N7-C8    | 2.45  | 107.31      | 103.45   |
| 3   | C     | 501  | ATP  | C5-N7-C8    | 2.44  | 107.28      | 103.45   |
| 3   | B     | 501  | ATP  | C5-N7-C8    | 2.42  | 107.26      | 103.45   |
| 3   | D     | 501  | ATP  | C5-N7-C8    | 2.42  | 107.26      | 103.45   |
| 5   | E     | 2001 | ADP  | C5-N7-C8    | 2.40  | 107.22      | 103.45   |
| 5   | H     | 2001 | ADP  | C5-N7-C8    | 2.39  | 107.21      | 103.45   |
| 3   | A     | 501  | ATP  | C5-N7-C8    | 2.38  | 107.19      | 103.45   |
| 5   | G     | 2001 | ADP  | C5-N7-C8    | 2.38  | 107.19      | 103.45   |
| 5   | F     | 2001 | ADP  | C5-N7-C8    | 2.35  | 107.14      | 103.45   |
| 3   | E     | 2004 | ATP  | C3'-C2'-C1' | 2.24  | 105.69      | 101.46   |
| 3   | H     | 2004 | ATP  | C3'-C2'-C1' | 2.23  | 105.69      | 101.46   |
| 3   | F     | 2004 | ATP  | C3'-C2'-C1' | 2.23  | 105.68      | 101.46   |
| 3   | G     | 2004 | ATP  | C3'-C2'-C1' | 2.22  | 105.67      | 101.46   |
| 3   | D     | 501  | ATP  | C2'-C1'-N9  | -2.20 | 107.83      | 113.30   |
| 3   | D     | 501  | ATP  | N9-C8-N7    | -2.12 | 110.93      | 113.94   |
| 3   | H     | 2004 | ATP  | N9-C8-N7    | -2.11 | 110.94      | 113.94   |
| 3   | G     | 2004 | ATP  | N9-C8-N7    | -2.10 | 110.96      | 113.94   |
| 3   | C     | 501  | ATP  | C2'-C1'-N9  | -2.10 | 108.10      | 113.30   |
| 3   | D     | 501  | ATP  | C6-C5-N7    | 2.07  | 136.08      | 132.09   |
| 3   | E     | 2004 | ATP  | N9-C8-N7    | -2.06 | 111.01      | 113.94   |
| 3   | E     | 2004 | ATP  | C2'-C1'-N9  | -2.06 | 108.18      | 113.30   |
| 3   | G     | 2004 | ATP  | C2'-C1'-N9  | -2.06 | 108.19      | 113.30   |
| 5   | F     | 2001 | ADP  | C3'-C2'-C1' | 2.06  | 105.36      | 101.46   |
| 5   | E     | 2001 | ADP  | C3'-C2'-C1' | 2.06  | 105.36      | 101.46   |
| 5   | H     | 2001 | ADP  | C3'-C2'-C1' | 2.05  | 105.35      | 101.46   |
| 3   | F     | 2004 | ATP  | C2'-C1'-N9  | -2.05 | 108.20      | 113.30   |
| 5   | G     | 2001 | ADP  | C3'-C2'-C1' | 2.05  | 105.34      | 101.46   |
| 3   | F     | 2004 | ATP  | N9-C8-N7    | -2.05 | 111.03      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | H     | 2004 | ATP  | C2'-C1'-N9  | -2.04 | 108.22      | 113.30   |
| 3   | E     | 2004 | ATP  | O3G-PG-O2G  | 2.03  | 115.40      | 107.80   |
| 5   | F     | 2001 | ADP  | C6-C5-N7    | 2.03  | 136.00      | 132.09   |
| 3   | G     | 2004 | ATP  | O3G-PG-O2G  | 2.02  | 115.39      | 107.80   |
| 3   | F     | 2004 | ATP  | O3G-PG-O2G  | 2.02  | 115.39      | 107.80   |
| 3   | G     | 2004 | ATP  | C2'-C3'-C4' | 2.02  | 106.52      | 102.61   |
| 5   | H     | 2001 | ADP  | C6-C5-N7    | 2.02  | 135.98      | 132.09   |
| 3   | H     | 2004 | ATP  | O3G-PG-O2G  | 2.02  | 115.37      | 107.80   |
| 3   | A     | 501  | ATP  | O2A-PA-O1A  | 2.01  | 121.82      | 112.44   |
| 3   | B     | 501  | ATP  | C6-C5-N7    | 2.01  | 135.97      | 132.09   |
| 3   | H     | 2004 | ATP  | C2'-C3'-C4' | 2.01  | 106.50      | 102.61   |
| 3   | D     | 501  | ATP  | O2A-PA-O1A  | 2.00  | 121.77      | 112.44   |
| 5   | E     | 2001 | ADP  | C6-C5-N7    | 2.00  | 135.95      | 132.09   |
| 3   | E     | 2004 | ATP  | C2'-C3'-C4' | 2.00  | 106.47      | 102.61   |

There are no chirality outliers.

All (38) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | B     | 501  | ATP  | C5'-O5'-PA-O2A  |
| 3   | B     | 501  | ATP  | C5'-O5'-PA-O3A  |
| 5   | E     | 2001 | ADP  | C5'-O5'-PA-O1A  |
| 5   | E     | 2001 | ADP  | C5'-O5'-PA-O2A  |
| 5   | E     | 2001 | ADP  | O4'-C4'-C5'-O5' |
| 5   | E     | 2001 | ADP  | C3'-C4'-C5'-O5' |
| 5   | H     | 2001 | ADP  | C5'-O5'-PA-O1A  |
| 5   | H     | 2001 | ADP  | C5'-O5'-PA-O2A  |
| 5   | H     | 2001 | ADP  | O4'-C4'-C5'-O5' |
| 5   | H     | 2001 | ADP  | C3'-C4'-C5'-O5' |
| 5   | G     | 2001 | ADP  | C5'-O5'-PA-O1A  |
| 5   | G     | 2001 | ADP  | C5'-O5'-PA-O2A  |
| 5   | G     | 2001 | ADP  | O4'-C4'-C5'-O5' |
| 5   | G     | 2001 | ADP  | C3'-C4'-C5'-O5' |
| 5   | F     | 2001 | ADP  | C5'-O5'-PA-O1A  |
| 5   | F     | 2001 | ADP  | C5'-O5'-PA-O2A  |
| 5   | F     | 2001 | ADP  | O4'-C4'-C5'-O5' |
| 5   | F     | 2001 | ADP  | C3'-C4'-C5'-O5' |
| 3   | B     | 501  | ATP  | PG-O3B-PB-O1B   |
| 5   | E     | 2001 | ADP  | PB-O3A-PA-O1A   |
| 5   | H     | 2001 | ADP  | PB-O3A-PA-O1A   |
| 5   | G     | 2001 | ADP  | PB-O3A-PA-O1A   |
| 5   | F     | 2001 | ADP  | PB-O3A-PA-O1A   |

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*Continued from previous page...*

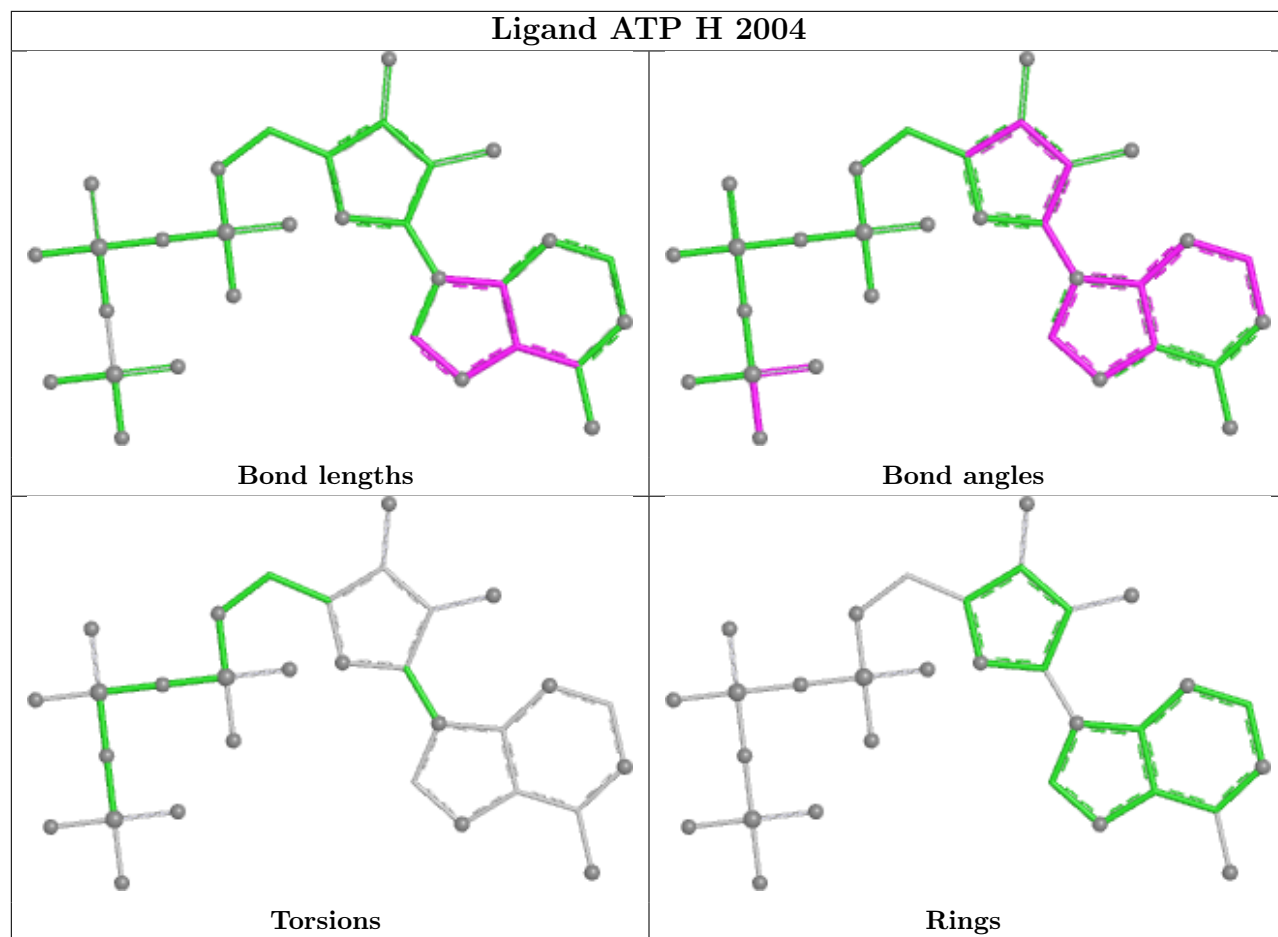
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | C     | 501  | ATP  | PG-O3B-PB-O2B   |
| 3   | D     | 501  | ATP  | PG-O3B-PB-O2B   |
| 3   | B     | 501  | ATP  | O4'-C4'-C5'-O5' |
| 5   | E     | 2001 | ADP  | C5'-O5'-PA-O3A  |
| 5   | H     | 2001 | ADP  | C5'-O5'-PA-O3A  |
| 5   | G     | 2001 | ADP  | C5'-O5'-PA-O3A  |
| 5   | F     | 2001 | ADP  | C5'-O5'-PA-O3A  |
| 3   | B     | 501  | ATP  | PG-O3B-PB-O2B   |
| 3   | D     | 501  | ATP  | PG-O3B-PB-O1B   |
| 5   | E     | 2001 | ADP  | PB-O3A-PA-O2A   |
| 5   | H     | 2001 | ADP  | PB-O3A-PA-O2A   |
| 5   | G     | 2001 | ADP  | PB-O3A-PA-O2A   |
| 5   | F     | 2001 | ADP  | PB-O3A-PA-O2A   |
| 3   | D     | 501  | ATP  | O4'-C4'-C5'-O5' |
| 3   | C     | 501  | ATP  | PG-O3B-PB-O1B   |

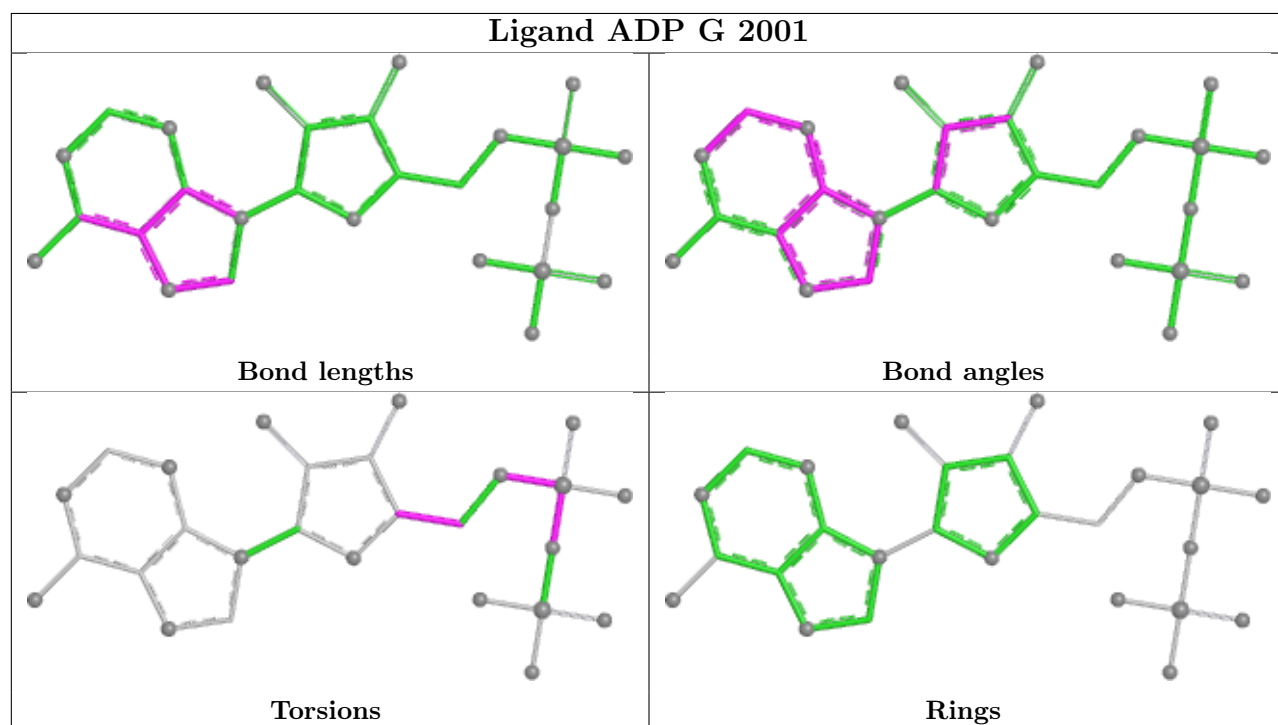
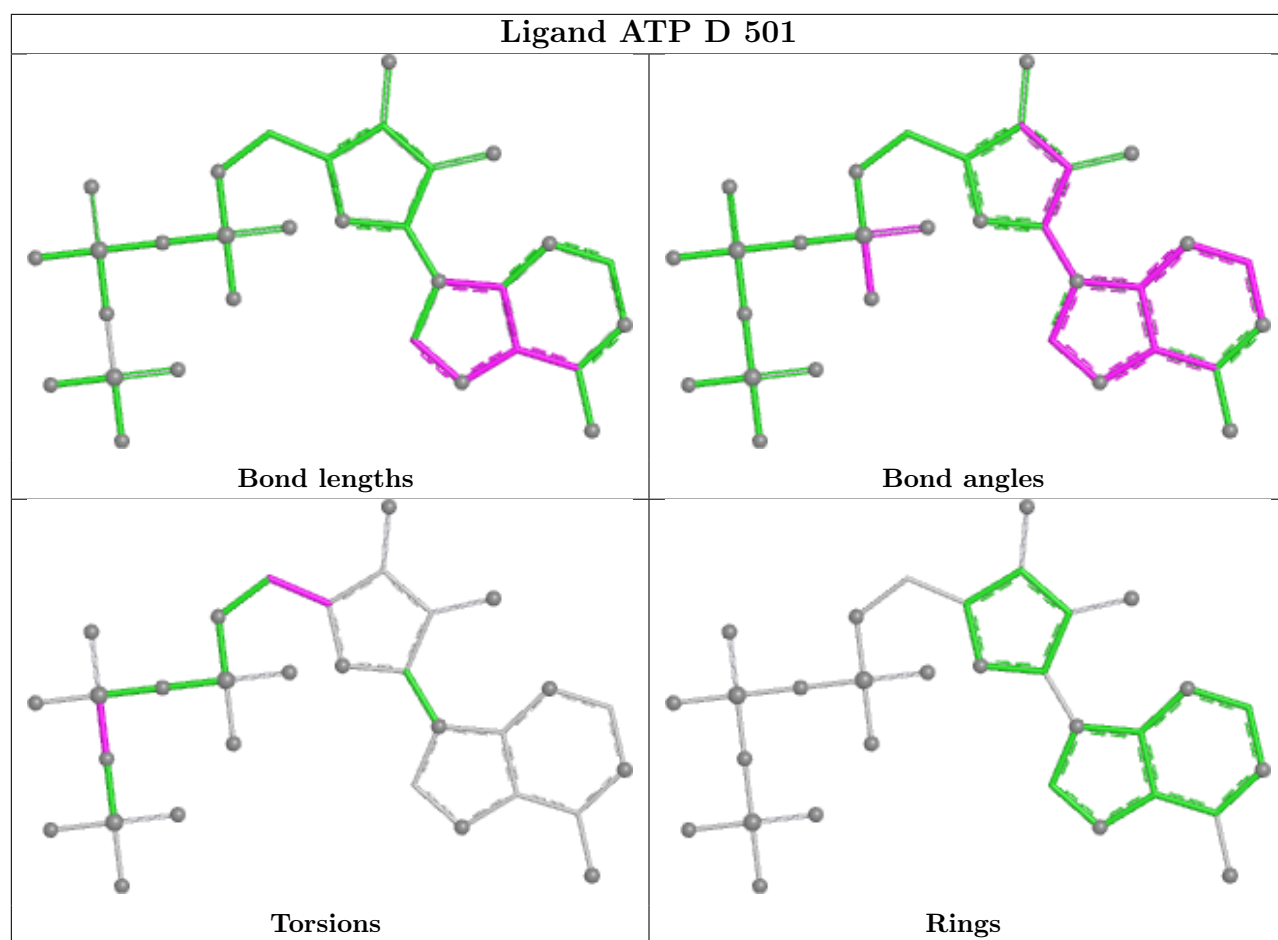
There are no ring outliers.

8 monomers are involved in 13 short contacts:

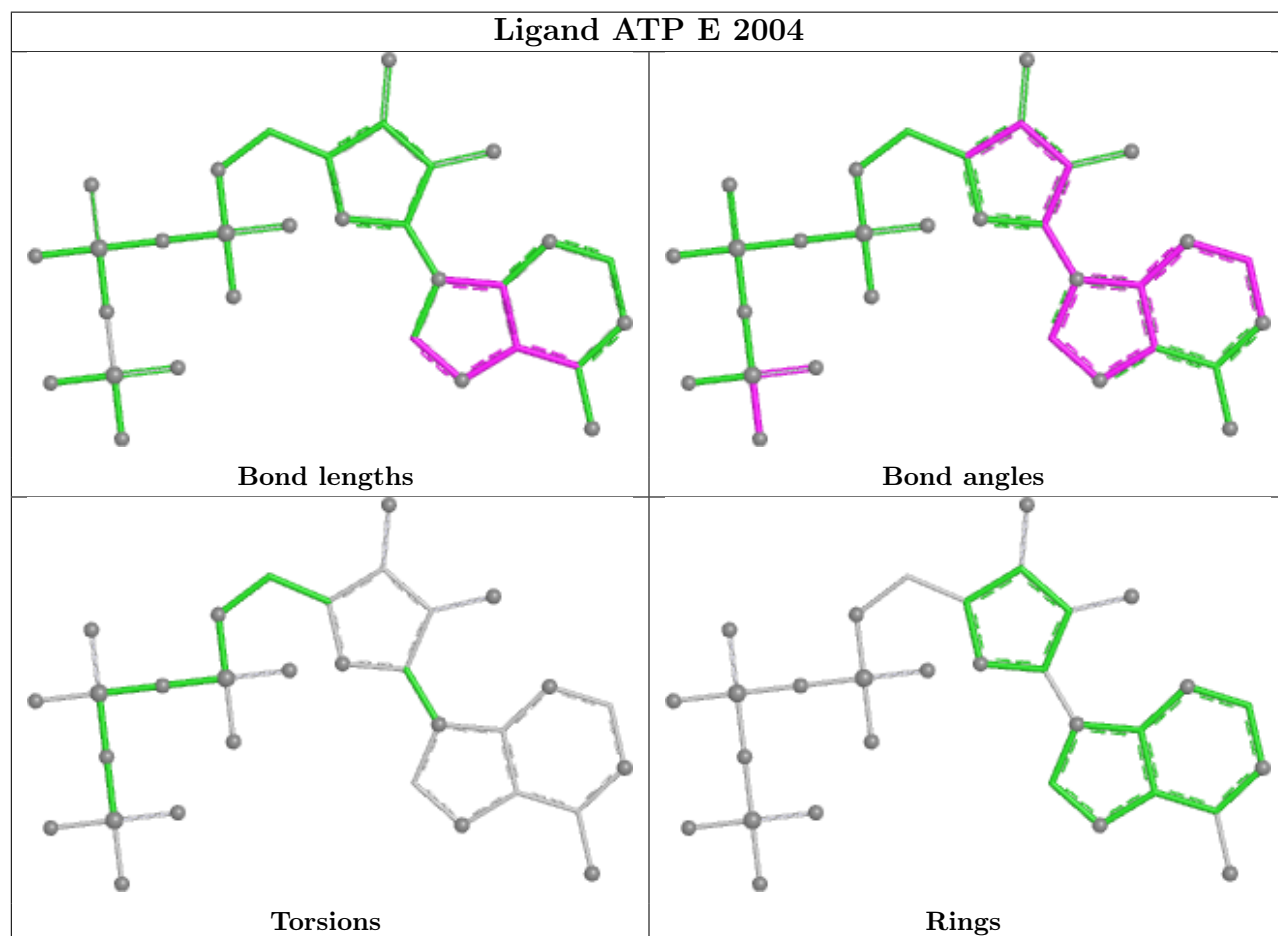
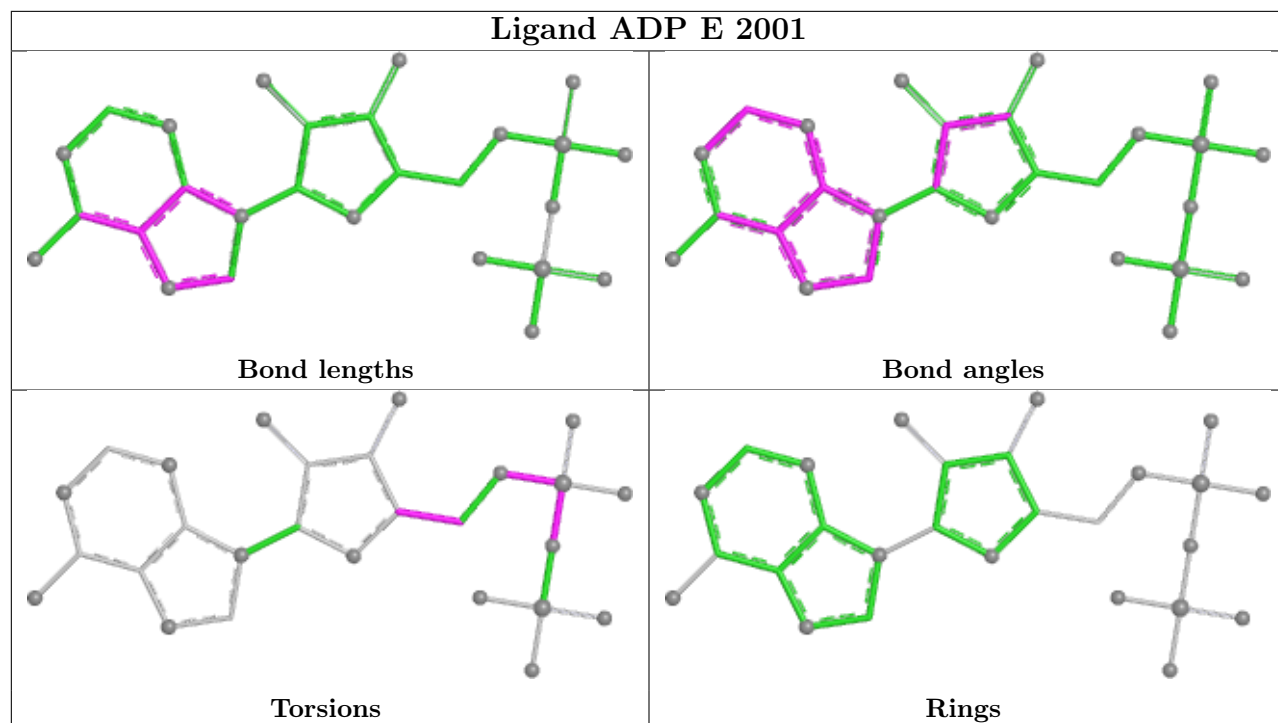
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | H     | 2004 | ATP  | 2       | 0            |
| 3   | D     | 501  | ATP  | 1       | 0            |
| 3   | E     | 2004 | ATP  | 2       | 0            |
| 3   | F     | 2004 | ATP  | 2       | 0            |
| 3   | A     | 501  | ATP  | 1       | 0            |
| 3   | G     | 2004 | ATP  | 3       | 0            |
| 3   | B     | 501  | ATP  | 1       | 0            |
| 3   | C     | 501  | ATP  | 1       | 0            |

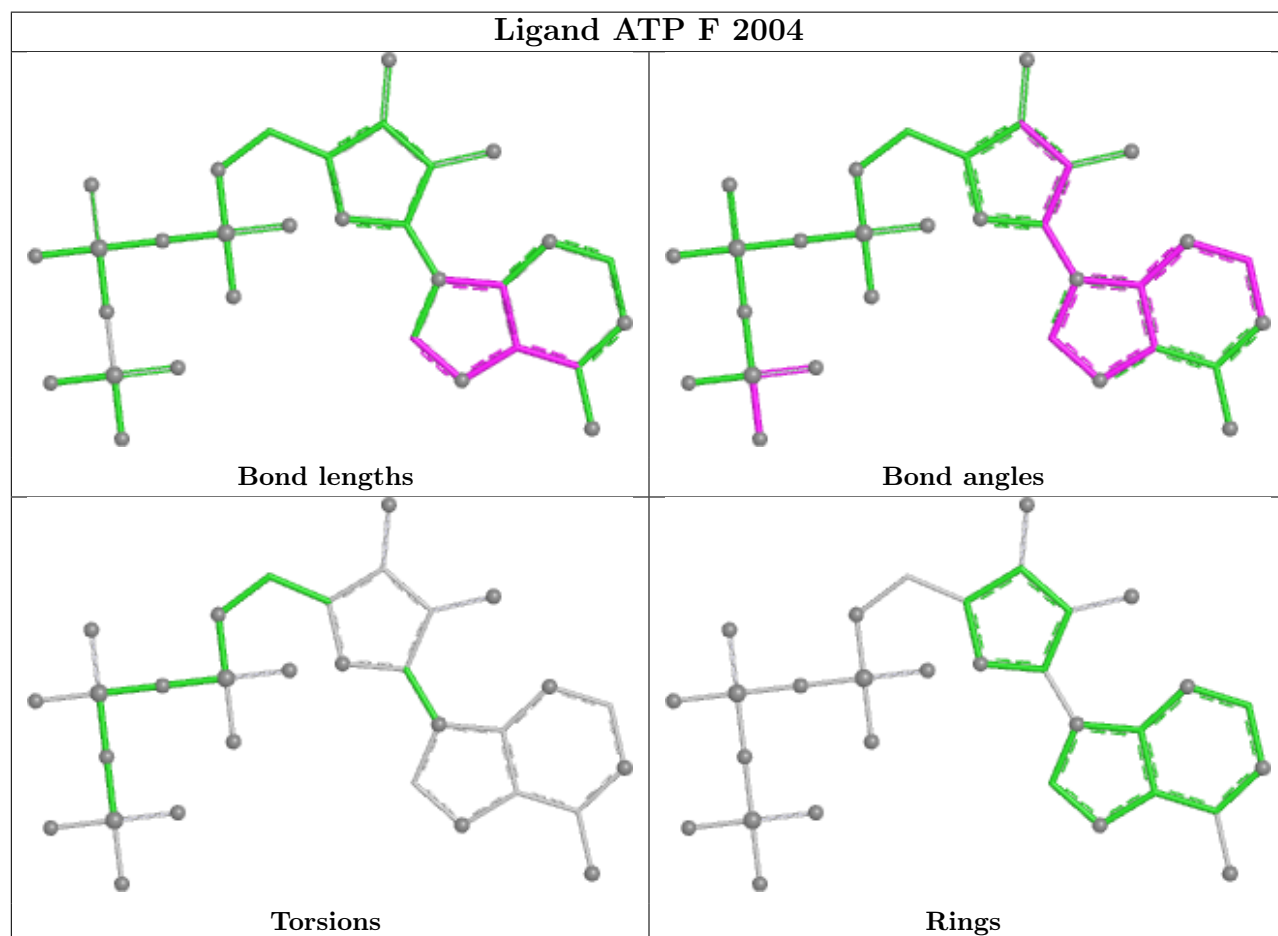
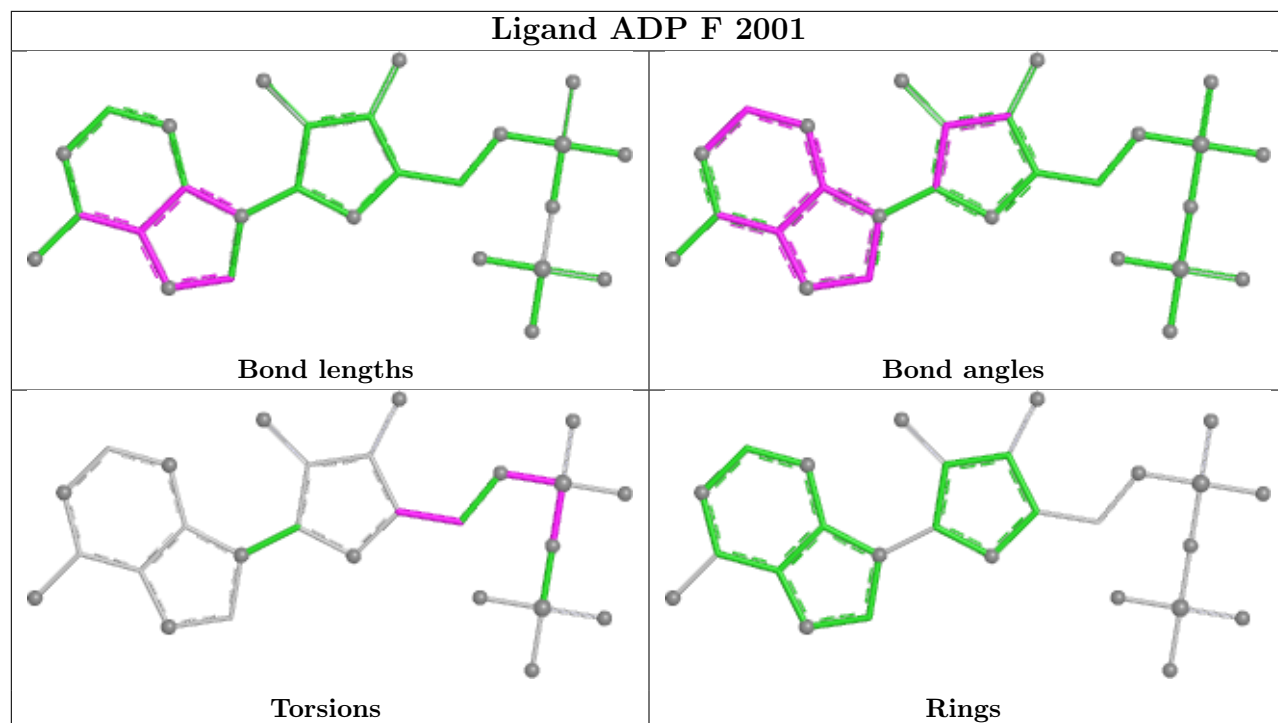
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

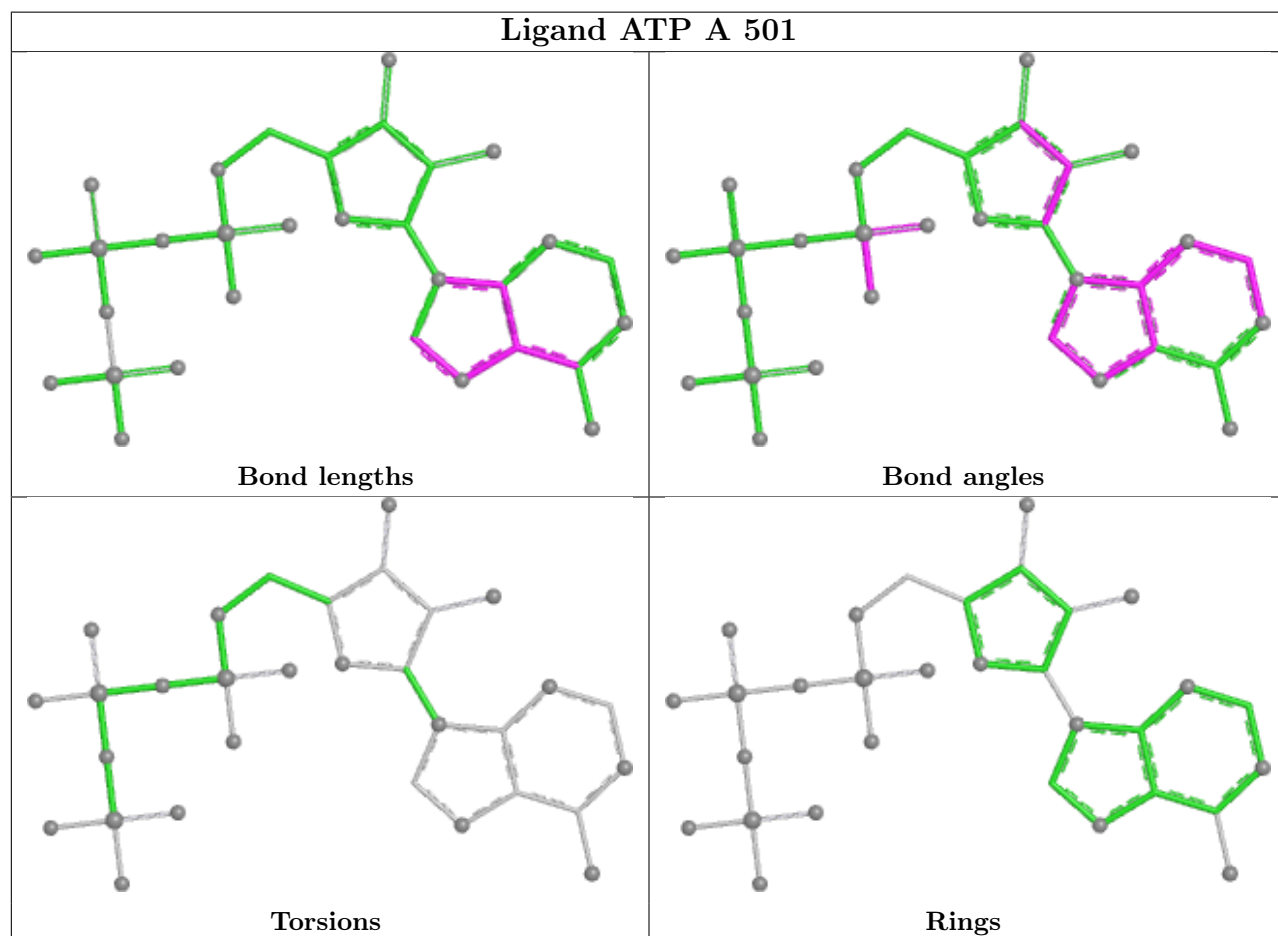
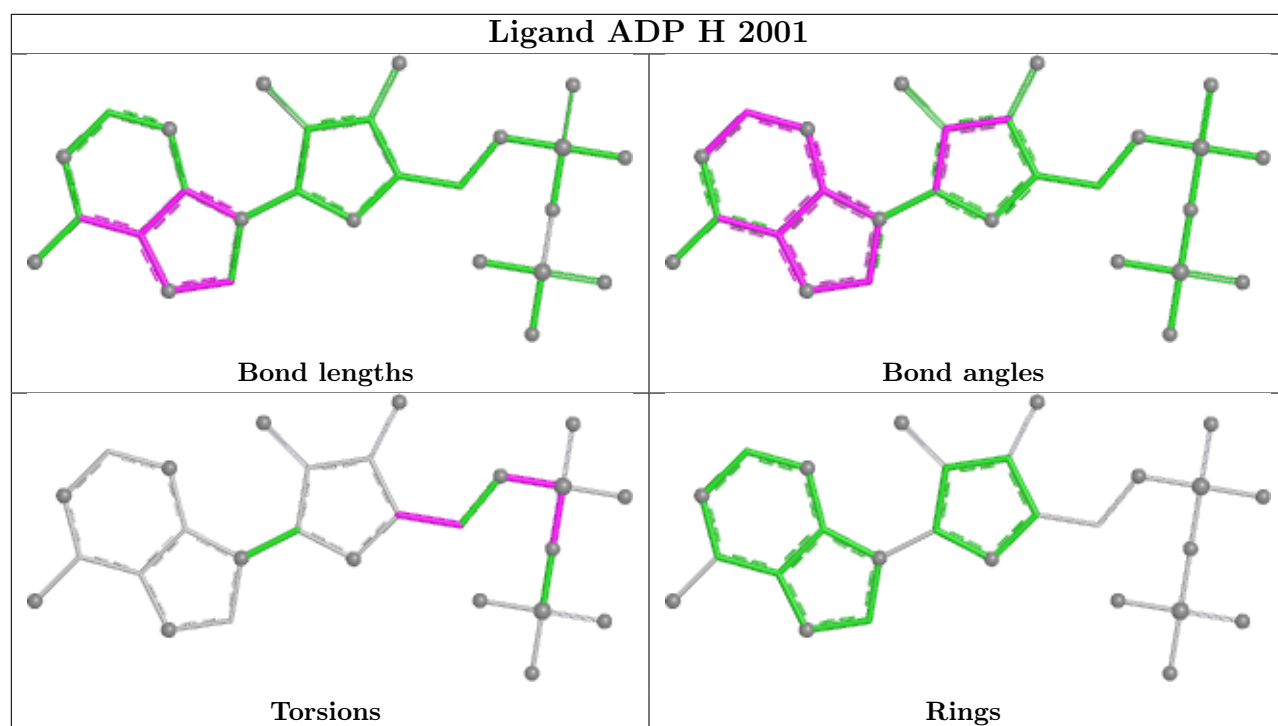


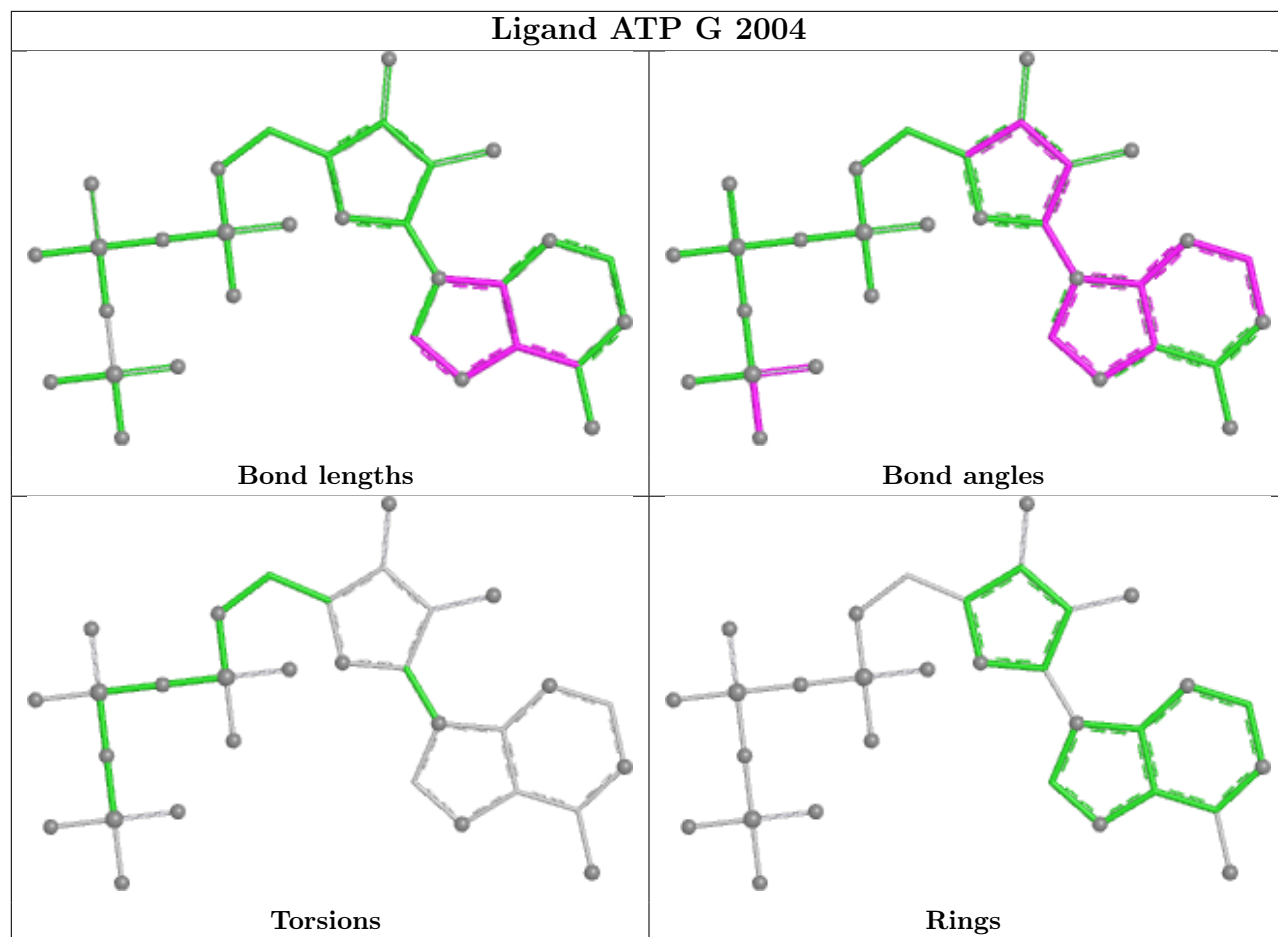


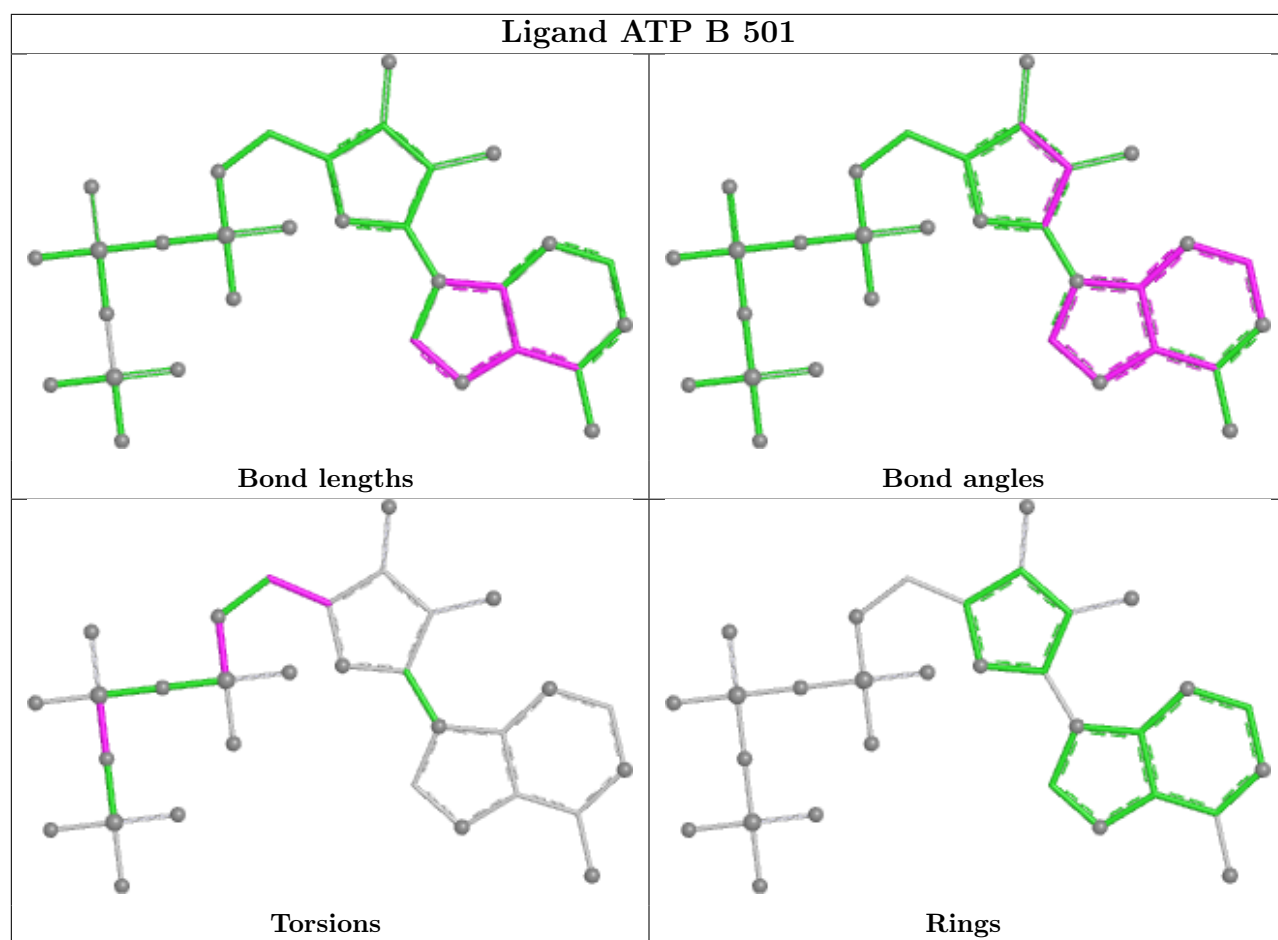


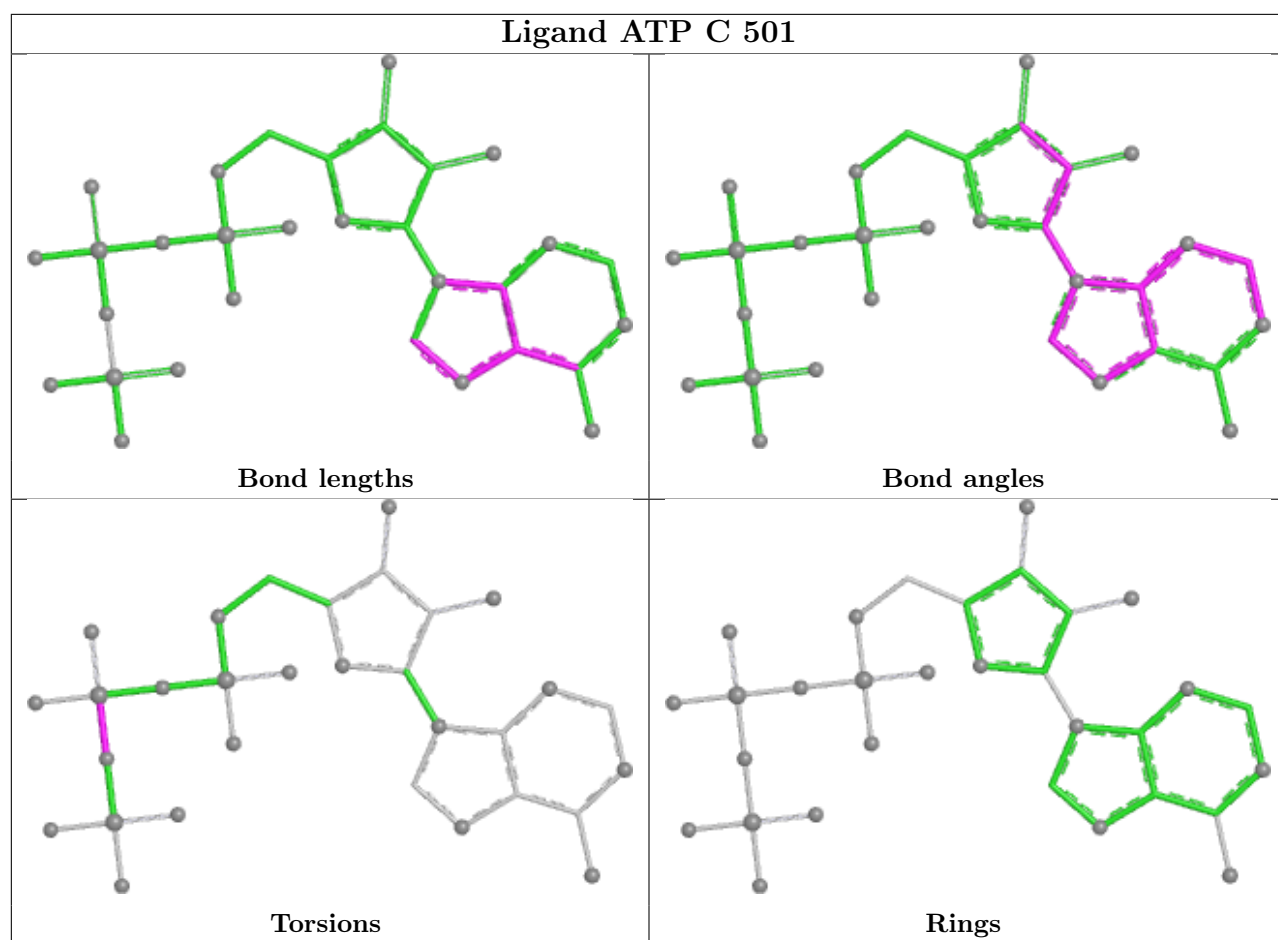












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

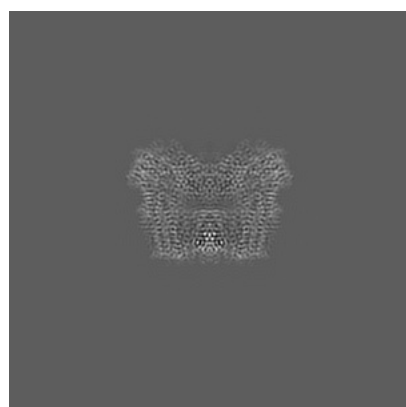
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7338. These allow visual inspection of the internal detail of the map and identification of artifacts.

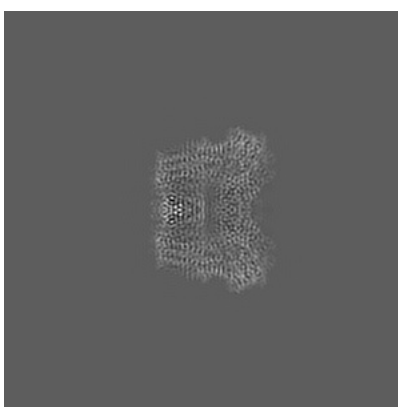
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

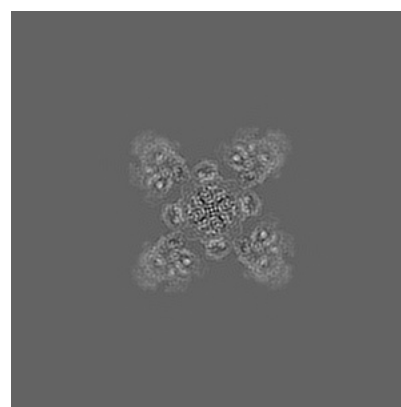
#### 6.1.1 Primary map



X



Y

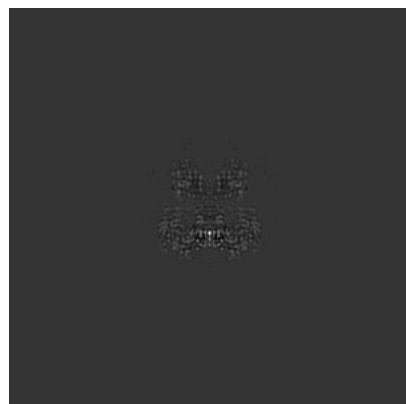


Z

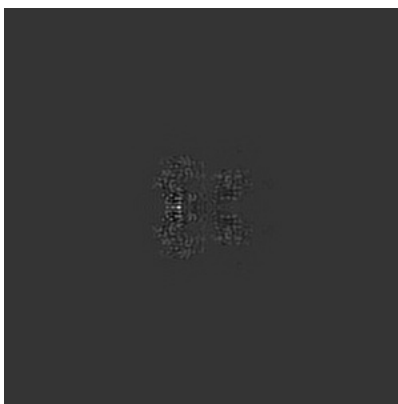
The images above show the map projected in three orthogonal directions.

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

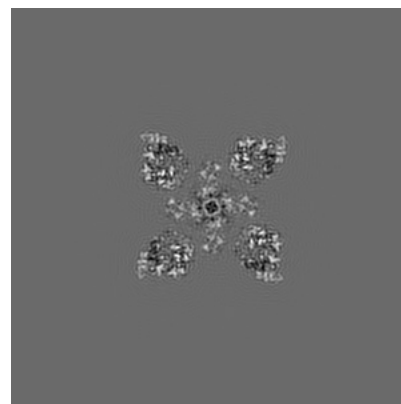
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

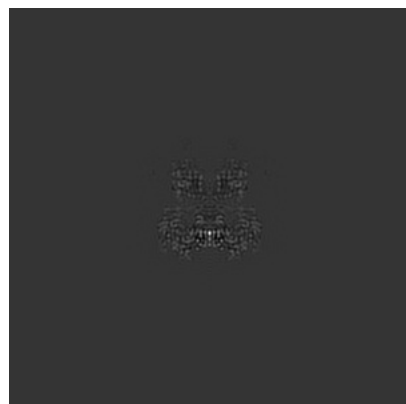


Z Index: 150

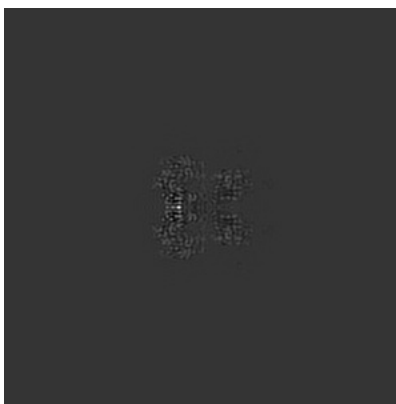
The images above show central slices of the map in three orthogonal directions.

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

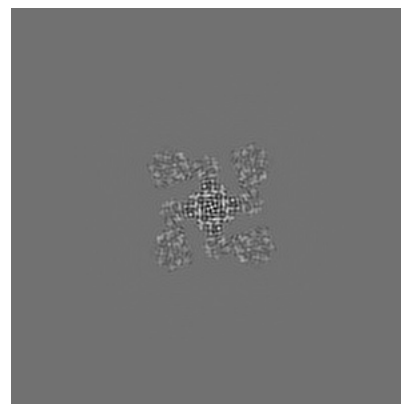
### 6.3.1 Primary map



X Index: 150



Y Index: 150

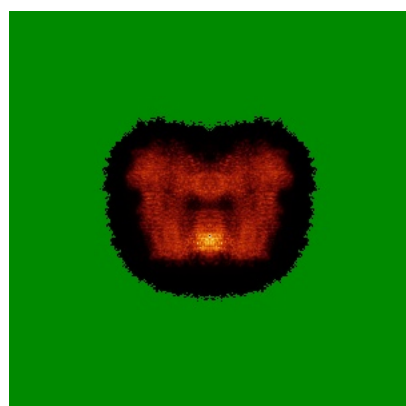


Z Index: 126

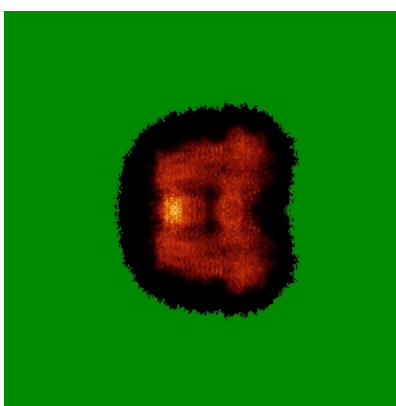
The images above show the largest variance slices of the map in three orthogonal directions.

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

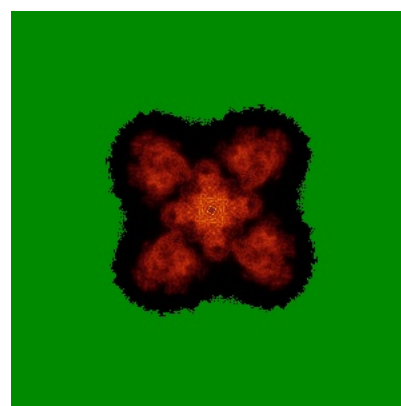
### 6.4.1 Primary map



X



Y



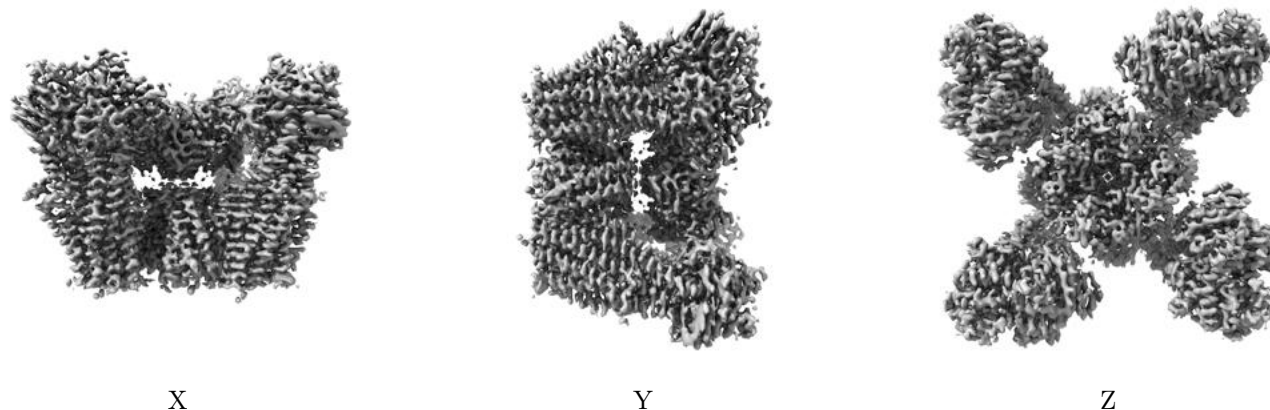
Z

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

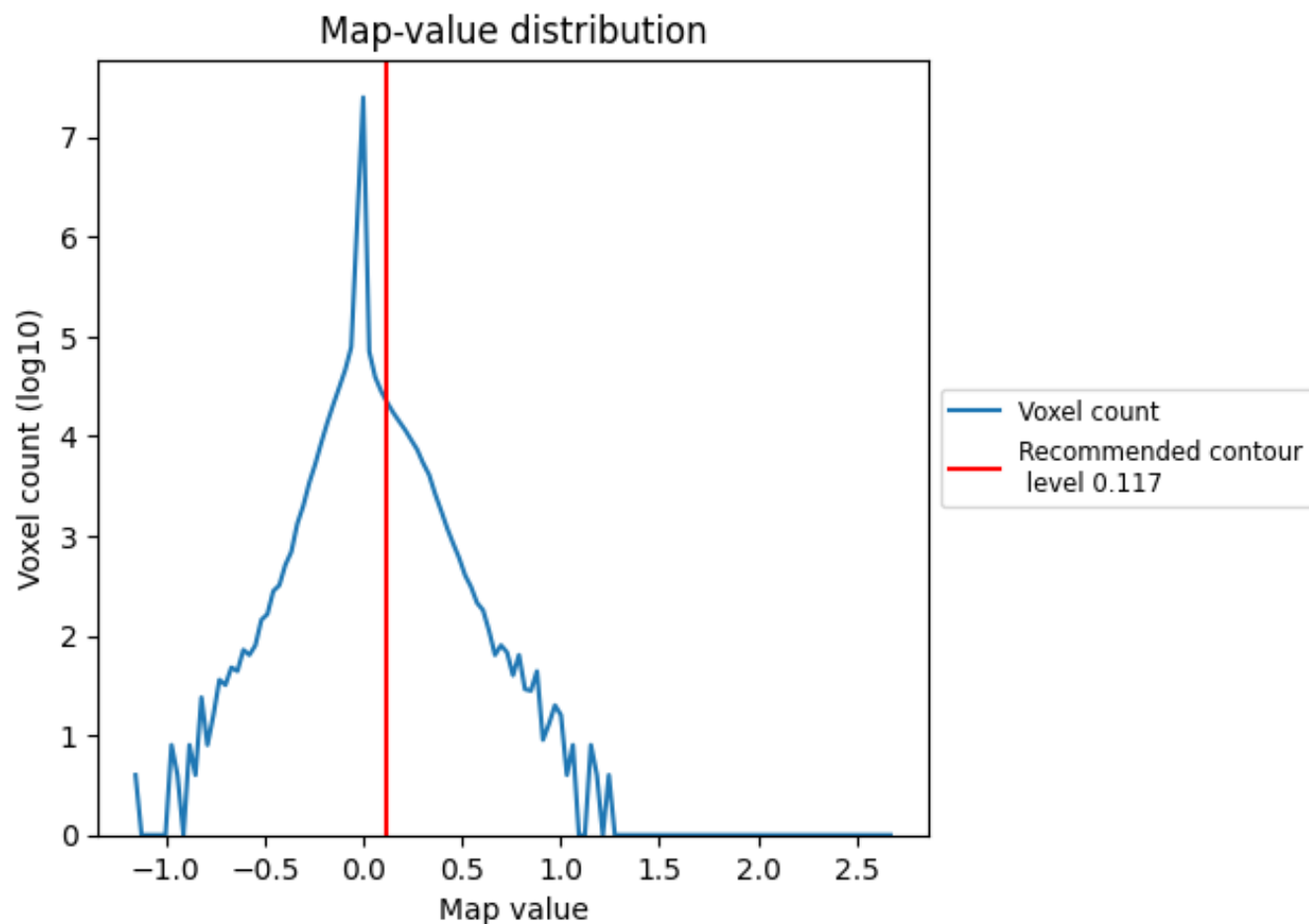
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

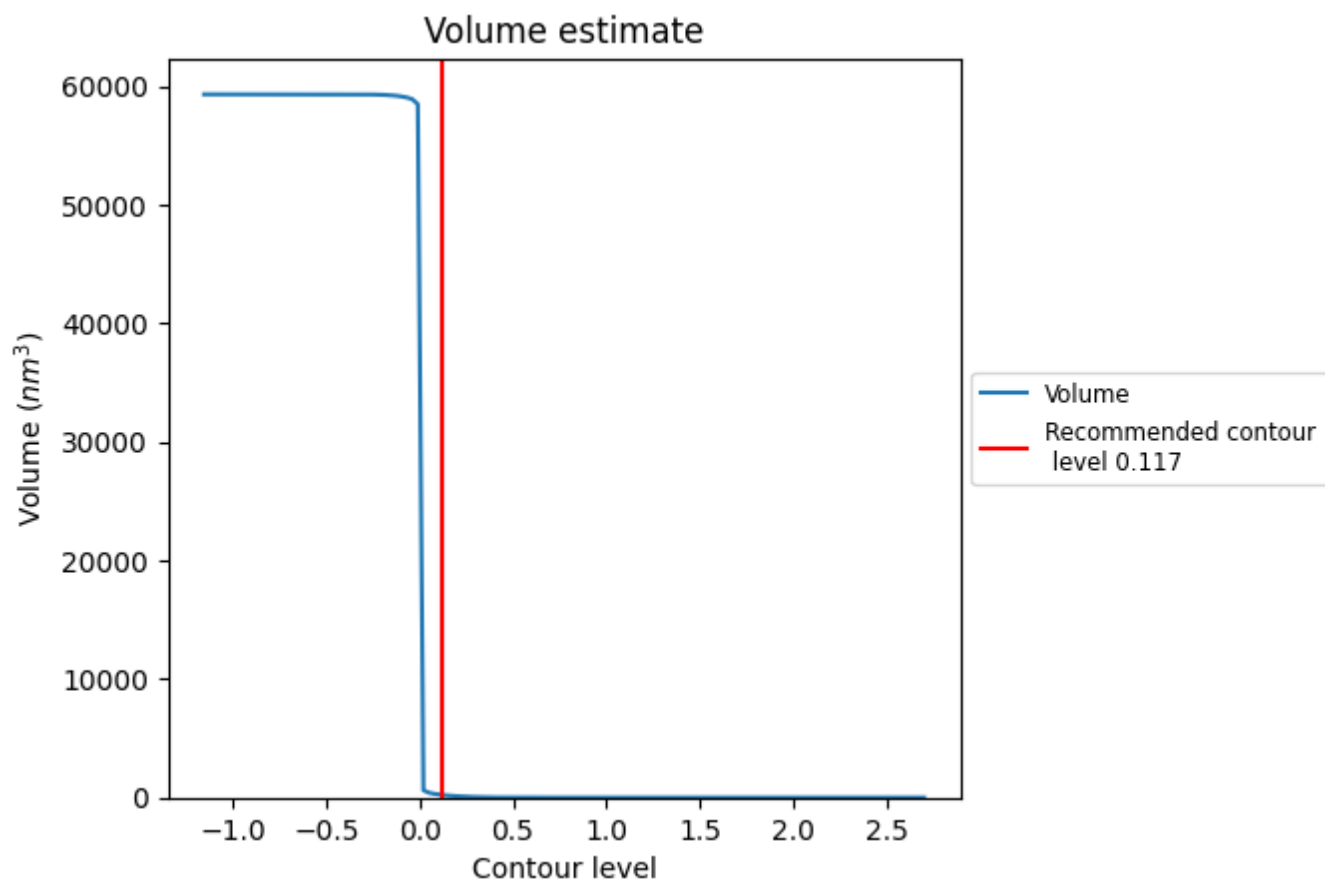
This section contains the results of statistical analysis of the map.

### 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.

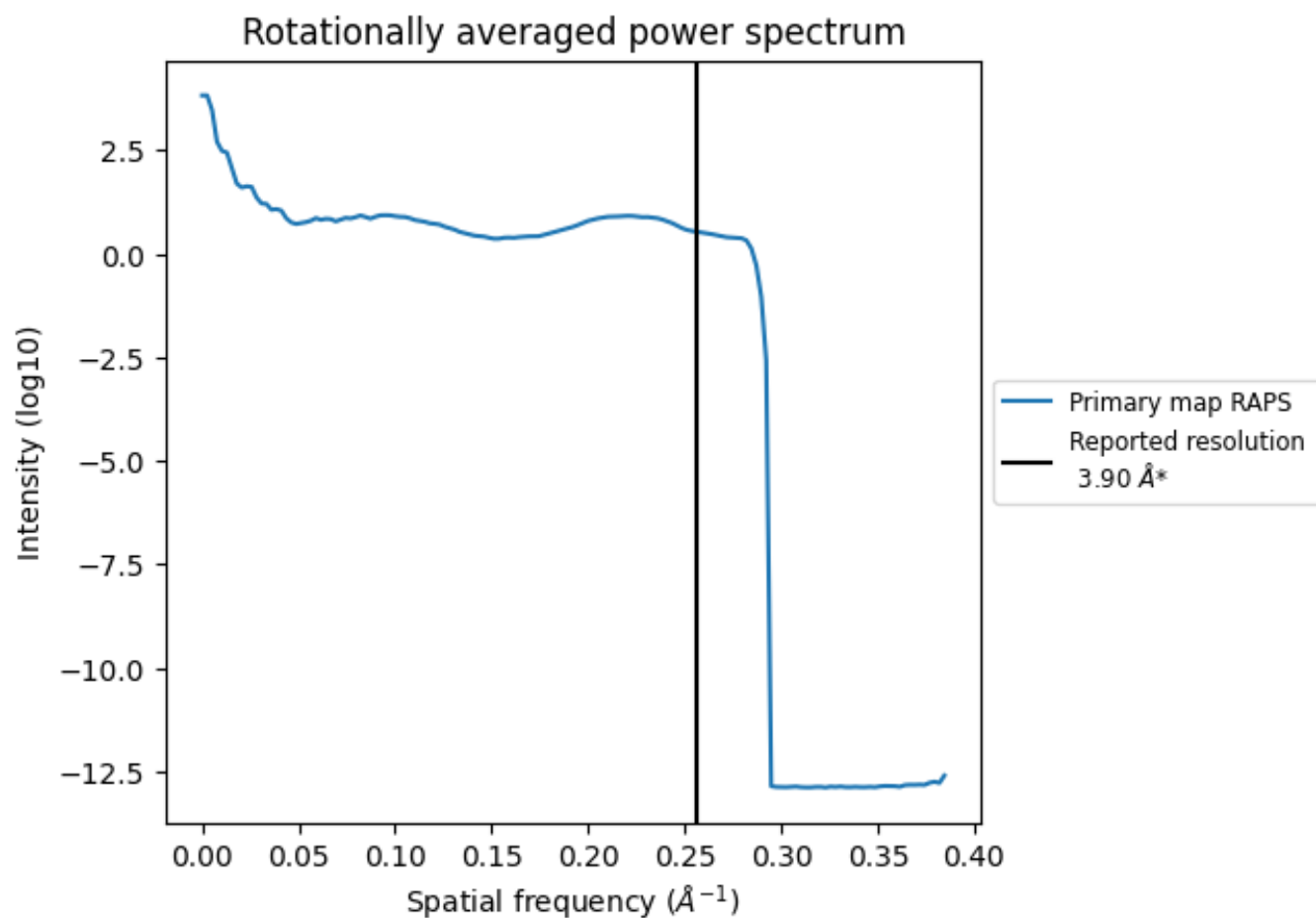
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227  $\text{nm}^3$ ; this corresponds to an approximate mass of 205 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 0.256 Å<sup>-1</sup>

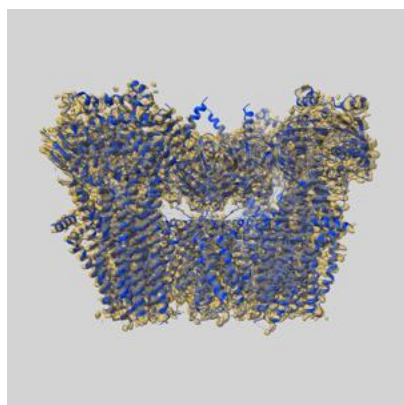
## 8 Fourier-Shell correlation ⓘ

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

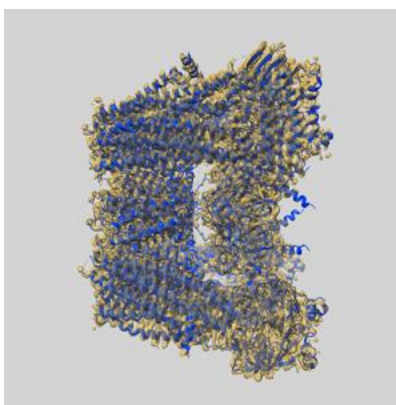
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7338 and PDB model 6C3O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

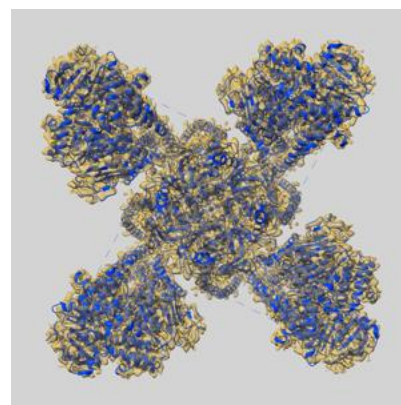
### 9.1 Map-model overlay [i](#)



X



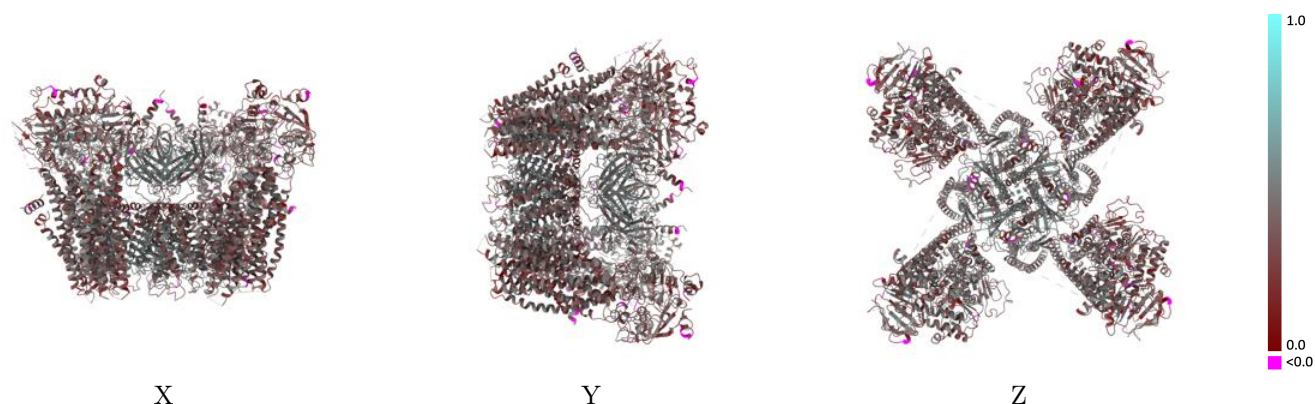
Y



Z

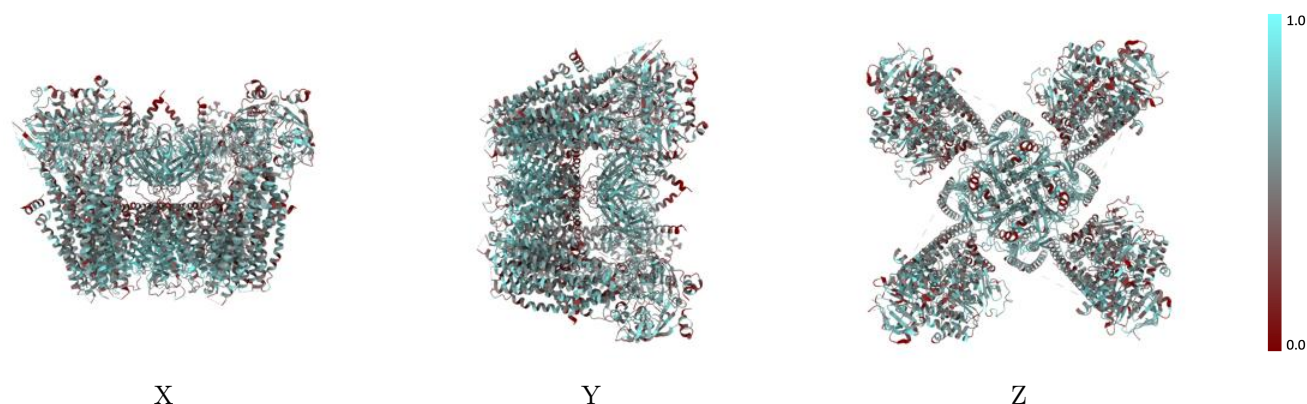
The images above show the 3D surface view of the map at the recommended contour level 0.117 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



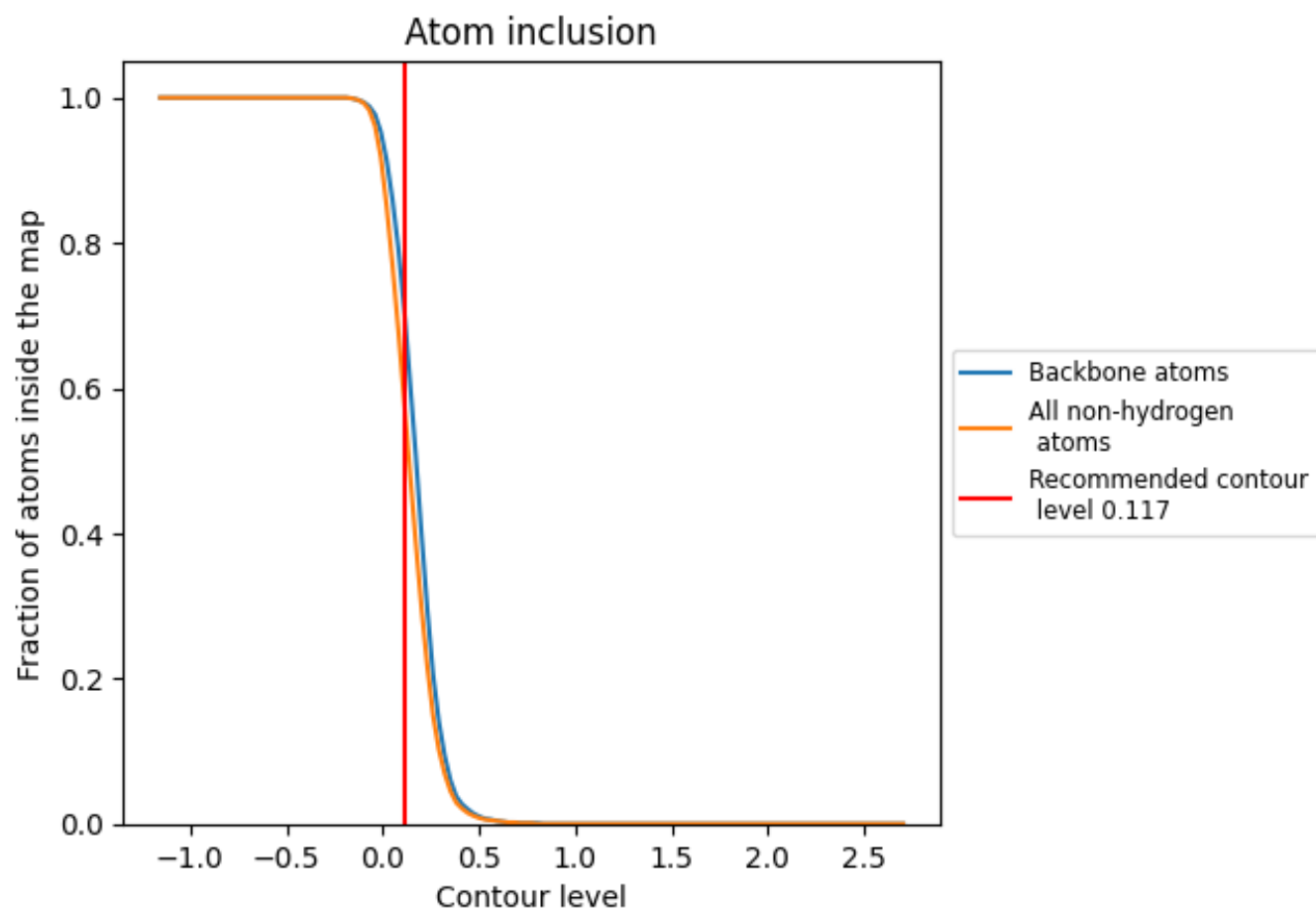
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.117).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 56% 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 (0.117) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.5640</div> | <div><div></div>0.3790</div> |
| A     | <div><div></div>0.6580</div> | <div><div></div>0.4520</div> |
| B     | <div><div></div>0.6540</div> | <div><div></div>0.4500</div> |
| C     | <div><div></div>0.6510</div> | <div><div></div>0.4360</div> |
| D     | <div><div></div>0.6460</div> | <div><div></div>0.4450</div> |
| E     | <div><div></div>0.5590</div> | <div><div></div>0.3830</div> |
| F     | <div><div></div>0.5410</div> | <div><div></div>0.3570</div> |
| G     | <div><div></div>0.5350</div> | <div><div></div>0.3570</div> |
| H     | <div><div></div>0.5310</div> | <div><div></div>0.3490</div> |

1.0

0.0

<0.0