



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 09:54 AM UTC

PDB ID : 7BKC / pdb\_00007bkc  
EMDB ID : EMD-12209  
Title : Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (dimeric, composite structure)  
Authors : Pfeil-Gardiner, O.; Watanabe, T.; Shima, S.; Murphy, B.J.  
Deposited on : 2021-01-15  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

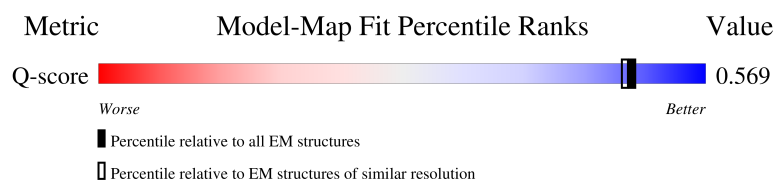
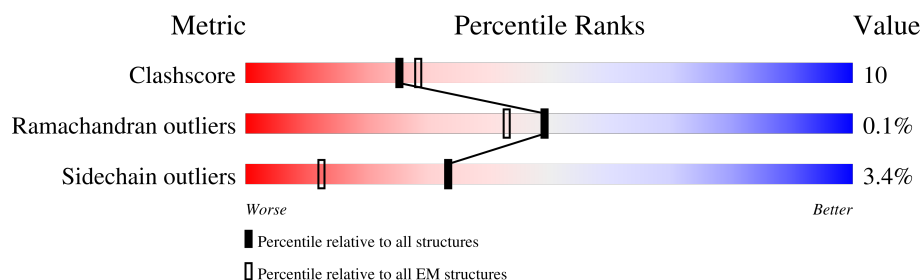
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.00 Å.

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



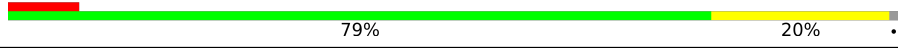
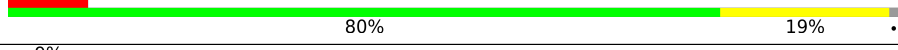
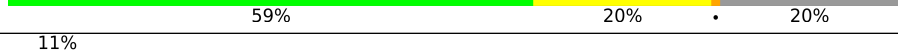
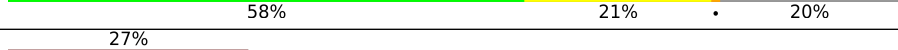
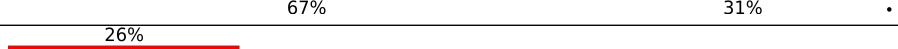
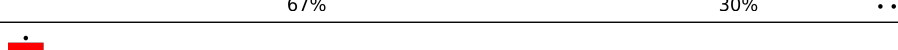
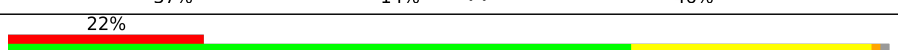
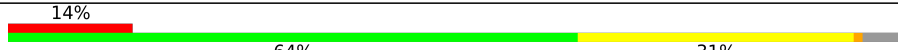
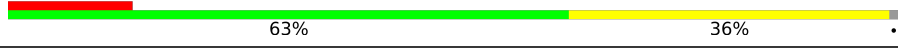
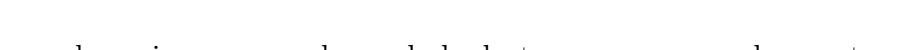
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14081 ( 2.50 - 3.50 )                                    |

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     | 671    |  |
| 1   | a     | 671    |  |
| 2   | F     | 140    |  |
| 2   | f     | 140    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | E     | 414    |    |
| 3   | e     | 414    |    |
| 4   | C     | 191    |    |
| 4   | c     | 191    |    |
| 5   | B     | 296    |    |
| 5   | b     | 296    |    |
| 6   | D     | 686    |    |
| 6   | d     | 686    |    |
| 7   | I     | 266    |    |
| 7   | i     | 266    |    |
| 8   | L     | 146    |    |
| 8   | l     | 146    |  |
| 9   | G     | 571    |  |
| 9   | g     | 571    |  |
| 10  | J     | 137    |  |
| 10  | j     | 137    |  |
| 11  | K     | 388    |  |
| 11  | M     | 388    |  |
| 11  | k     | 388    |  |
| 11  | m     | 388    |  |
| 12  | H     | 443    |  |
| 12  | h     | 443    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | SF4  | A     | 703 | -         | -        | X       | -                |
| 13  | SF4  | a     | 703 | -         | -        | X       | -                |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 64126 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 CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 662      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5011  | 3168 | 851 | 935 | 57 |         |       |
| 1   | a     | 662      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5011  | 3168 | 851 | 935 | 57 |         |       |

- Molecule 2 is a protein called F420-non-reducing hydrogenase subunit D.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | F     | 137      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1073  | 687 | 188 | 186 | 12 |         |       |
| 2   | f     | 137      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1073  | 687 | 188 | 186 | 12 |         |       |

- Molecule 3 is a protein called Formate dehydrogenase, beta subunit (F420).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | E     | 411      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3151  | 1985 | 542 | 589 | 35 |         |       |
| 3   | e     | 411      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3151  | 1985 | 542 | 589 | 35 |         |       |

- Molecule 4 is a protein called CoB–CoM heterodisulfide reductase subunit C.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | C     | 189      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1498  | 936 | 271 | 278 | 13 |         |       |
| 4   | c     | 189      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1498  | 936 | 271 | 278 | 13 |         |       |

- Molecule 5 is a protein called CoB–CoM heterodisulfide reductase subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | B     | 296      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2304  | 1470 | 387 | 426 | 21 |         |       |
| 5   | b     | 296      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2304  | 1470 | 387 | 426 | 21 |         |       |

- Molecule 6 is a protein called Formate dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | D     | 549      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4251  | 2691 | 737 | 795 | 28 |         |       |
| 6   | d     | 549      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4251  | 2691 | 737 | 795 | 28 |         |       |

- Molecule 7 is a protein called Formylmethanofuran dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | I     | 264      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1996  | 1270 | 336 | 380 | 10 |         |       |
| 7   | i     | 264      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1996  | 1270 | 336 | 380 | 10 |         |       |

- Molecule 8 is a protein called Formylmethanofuran dehydrogenase, subunit G.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 8   | L     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 576   | 357 | 98 | 112 | 9 |         |       |
| 8   | l     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 576   | 357 | 98 | 112 | 9 |         |       |

- Molecule 9 is a protein called Formylmethanofuran dehydrogenase, subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | G     | 568      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4455  | 2840 | 751 | 841 | 23 |         |       |
| 9   | g     | 568      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4455  | 2840 | 751 | 841 | 23 |         |       |

- Molecule 10 is a protein called Formylmethanofuran dehydrogenase, subunit D.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1007  | 629 | 179 | 190 | 9 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | j     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1007  | 629 | 179 | 190 | 9 |         |       |

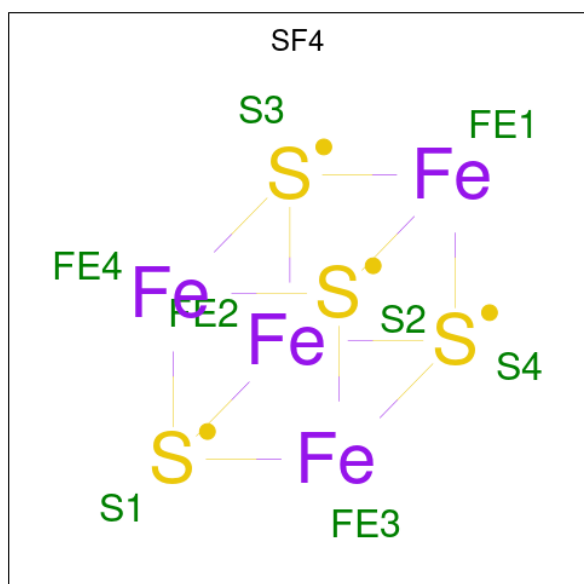
- Molecule 11 is a protein called Formylmethanofuran dehydrogenase, subunit F.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | M     | 65       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 487   | 303  | 77  | 99  | 8  |         |       |
| 11  | K     | 321      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2423  | 1512 | 411 | 472 | 28 |         |       |
| 11  | m     | 65       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 487   | 303  | 77  | 99  | 8  |         |       |
| 11  | k     | 321      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2423  | 1512 | 411 | 472 | 28 |         |       |

- Molecule 12 is a protein called Formylmethanofuran dehydrogenase, subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | H     | 438      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3416  | 2155 | 600 | 629 | 32 |         |       |
| 12  | h     | 438      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3416  | 2155 | 600 | 629 | 32 |         |       |

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | D     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | L     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | L     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | K     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | K     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | K     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 13  | K     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

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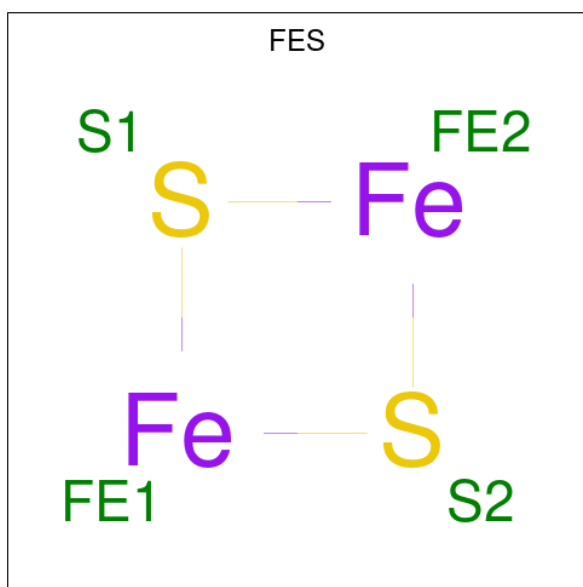
| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 13  | K     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | H     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | a     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | e     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | e     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | e     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | e     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | c     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | c     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | d     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | l     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | l     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | m     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | m     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |

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| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | k     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |
| 13  | h     | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       |

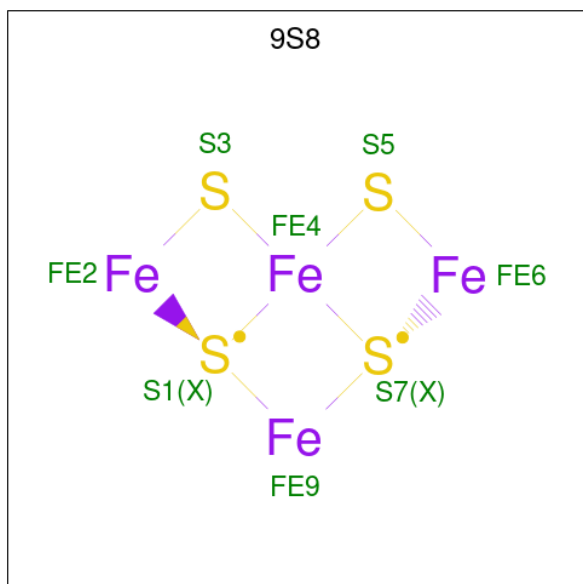
- # FAD

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | F     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 15  | f     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 16 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | b     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | b     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

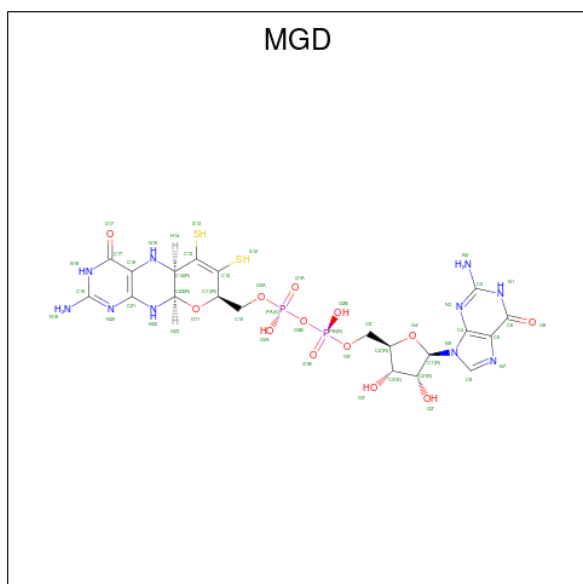
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | G     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 17  | g     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 18 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 18  | H     | 1        | Total | Mo | 0       |
|     |       |          | 1     | 1  |         |
| 18  | h     | 1        | Total | Mo | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 19 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

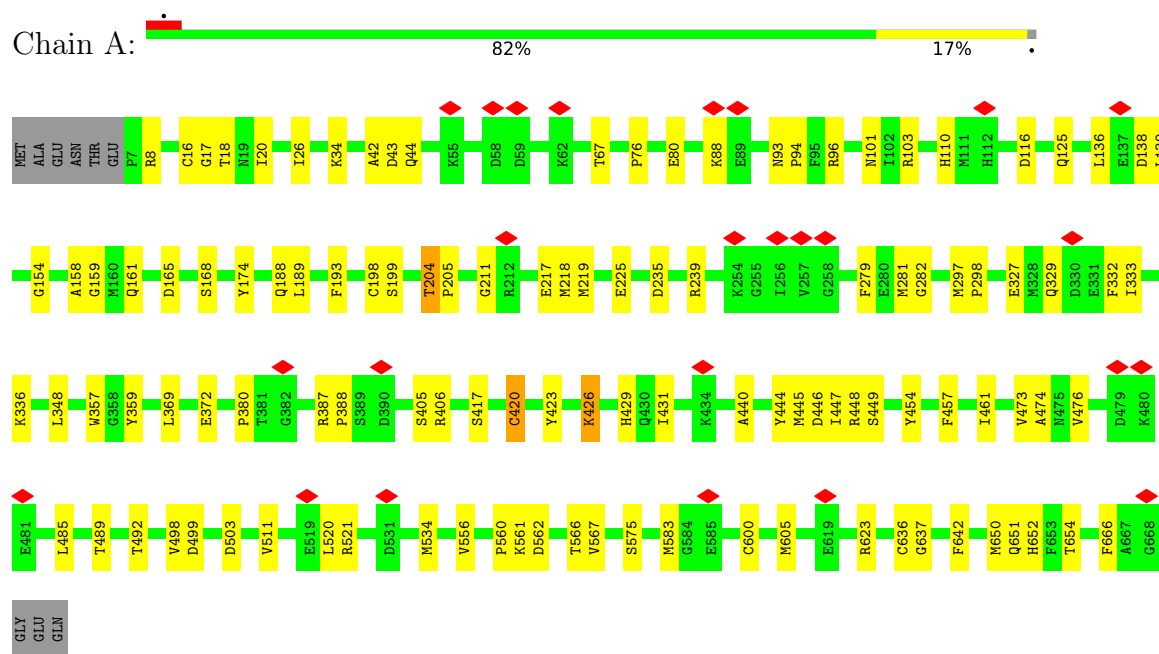


| Mol | Chain | Residues | Atoms       |         |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|--------|--------|---------|
| 19  | H     | 1        | Total<br>47 | C<br>20 | N<br>10 | O<br>13 | P<br>2 | S<br>2 | 0       |
| 19  | H     | 1        | Total<br>47 | C<br>20 | N<br>10 | O<br>13 | P<br>2 | S<br>2 | 0       |
| 19  | h     | 1        | Total<br>47 | C<br>20 | N<br>10 | O<br>13 | P<br>2 | S<br>2 | 0       |
| 19  | h     | 1        | Total<br>47 | C<br>20 | N<br>10 | O<br>13 | P<br>2 | S<br>2 | 0       |

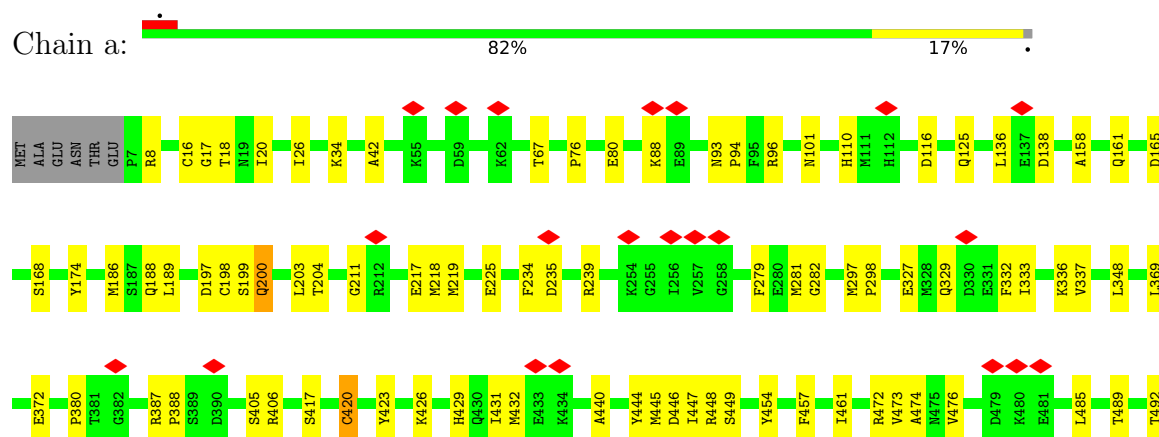
### 3 Residue-property plots

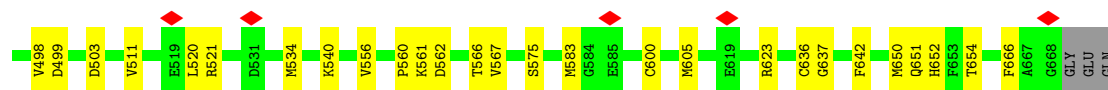
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

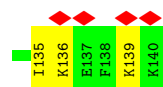
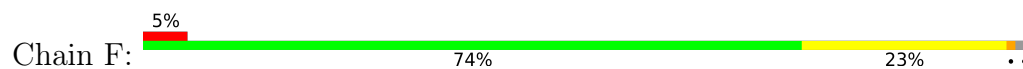


#### • Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

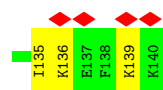
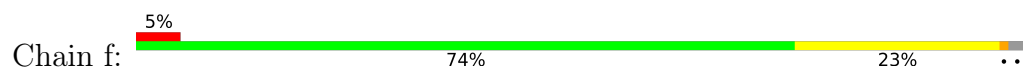




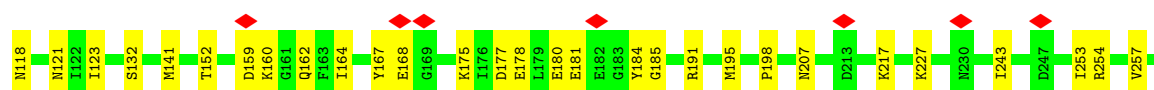
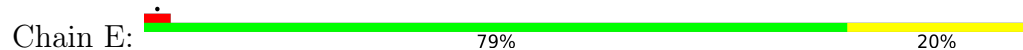
- Molecule 2: F420-non-reducing hydrogenase subunit D



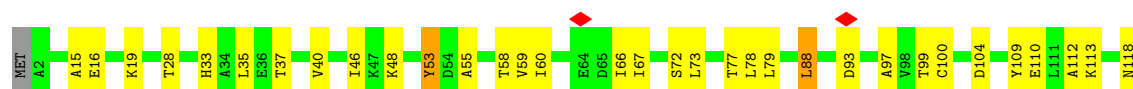
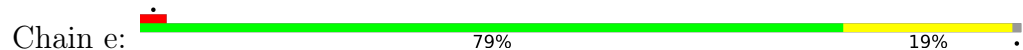
- Molecule 2: F420-non-reducing hydrogenase subunit D

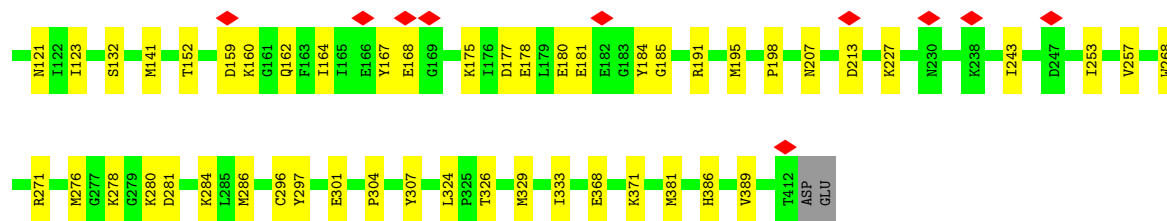


- Molecule 3: Formate dehydrogenase, beta subunit (F420)

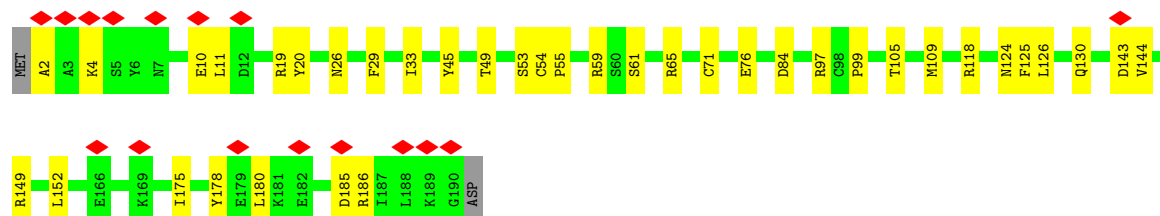


- Molecule 3: Formate dehydrogenase, beta subunit (F420)

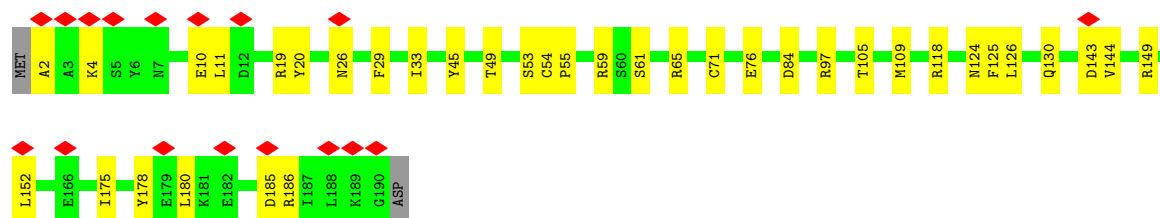
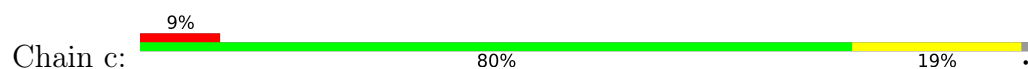




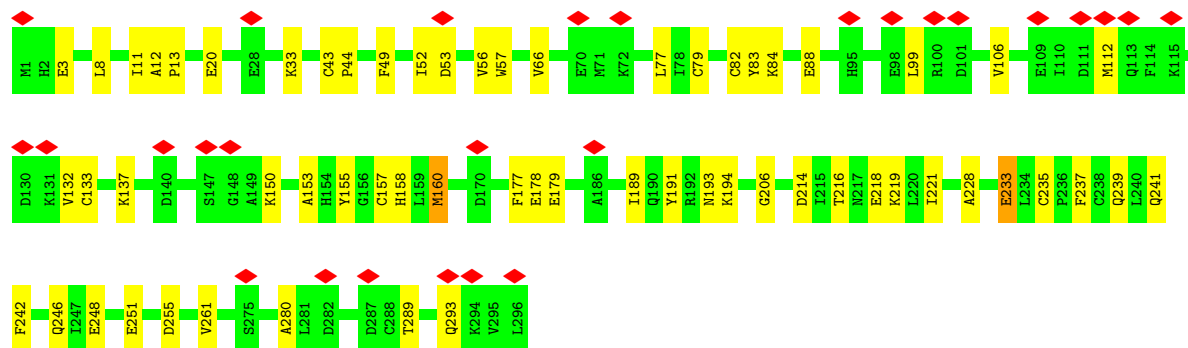
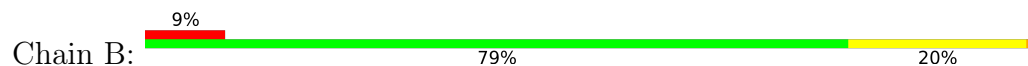
• Molecule 4: CoB–CoM heterodisulfide reductase subunit C



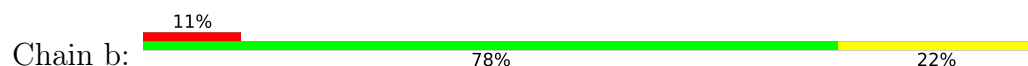
• Molecule 4: CoB–CoM heterodisulfide reductase subunit C



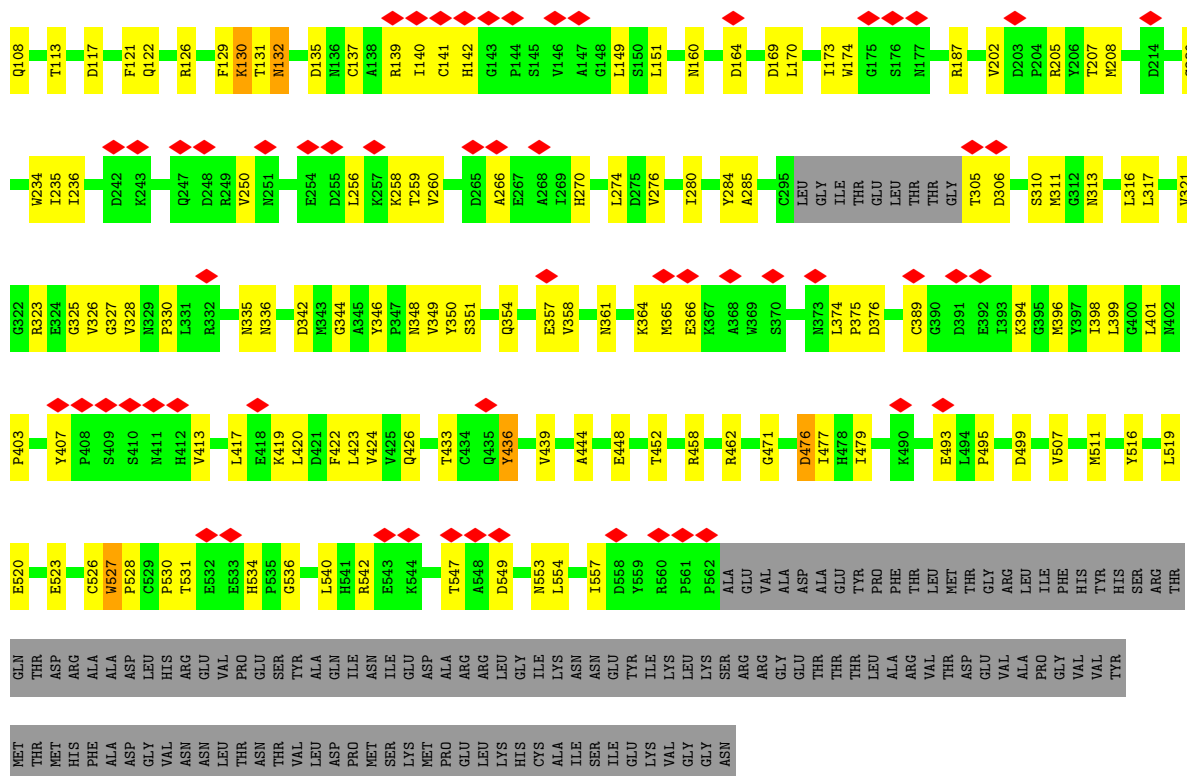
• Molecule 5: CoB–CoM heterodisulfide reductase subunit B



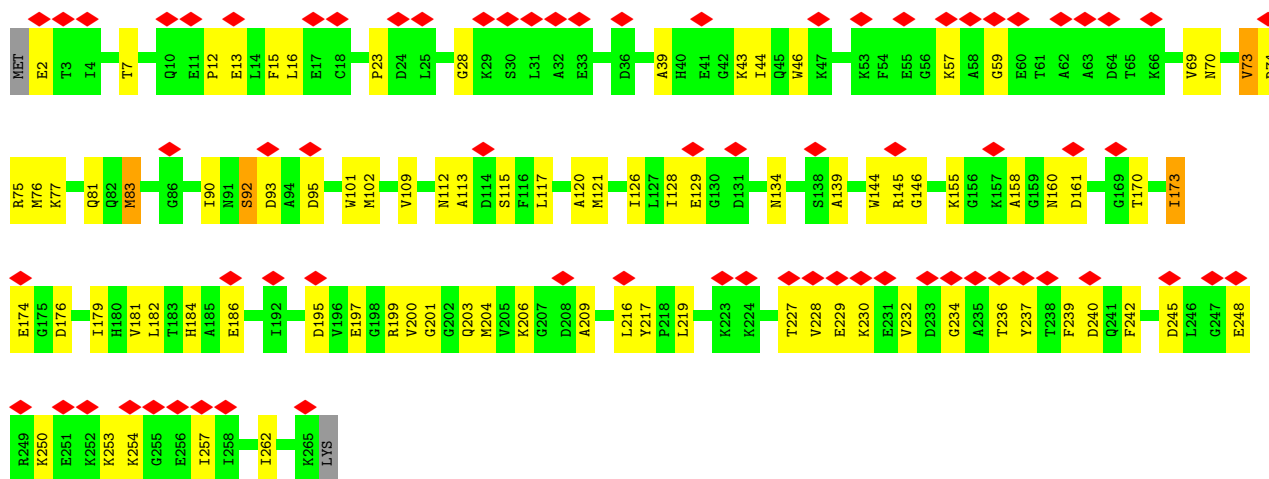
• Molecule 5: CoB–CoM heterodisulfide reductase subunit B



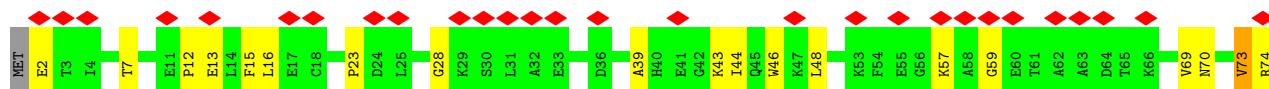


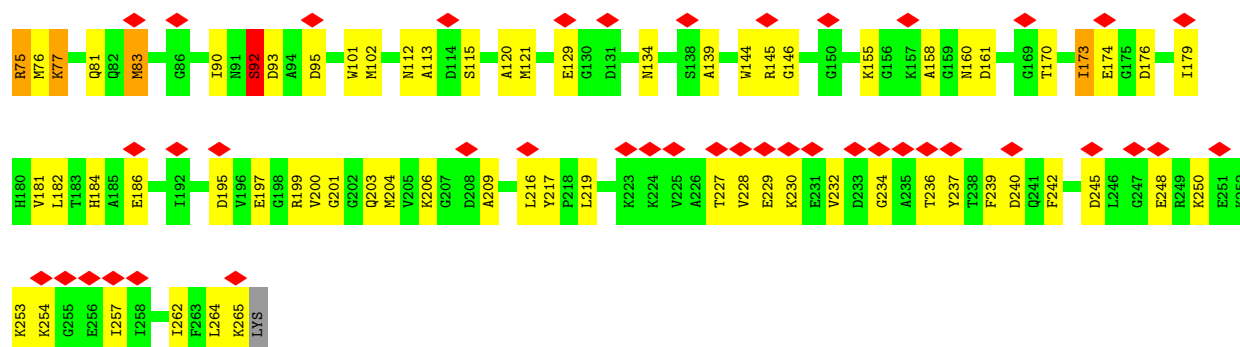


• Molecule 7: Formylmethanofuran dehydrogenase



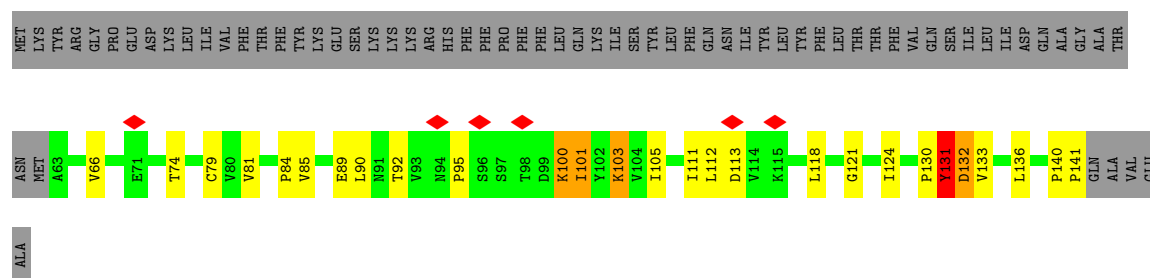
• Molecule 7: Formylmethanofuran dehydrogenase





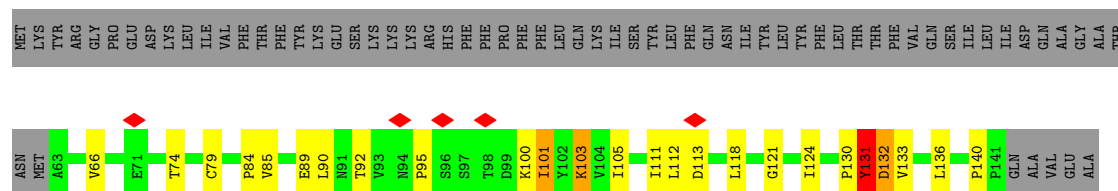
- Molecule 8: Formylmethanofuran dehydrogenase, subunit G

Chain L: 36% 15% 46%



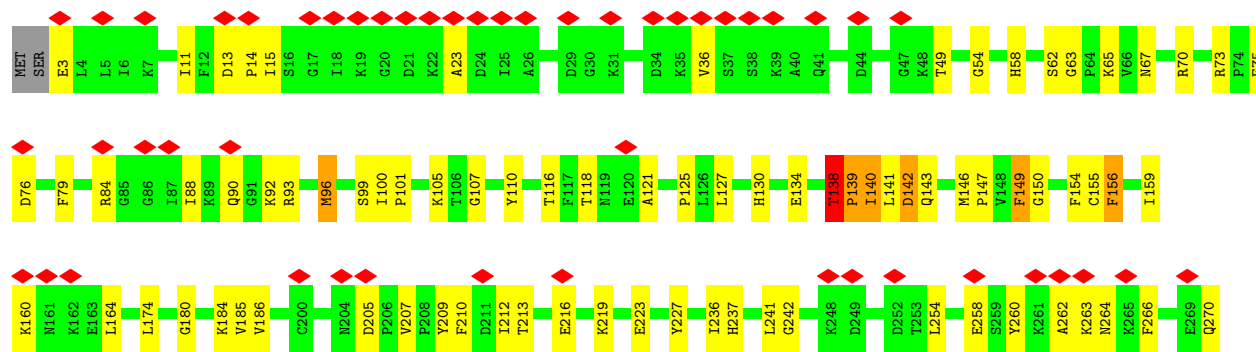
- Molecule 8: Formylmethanofuran dehydrogenase, subunit G

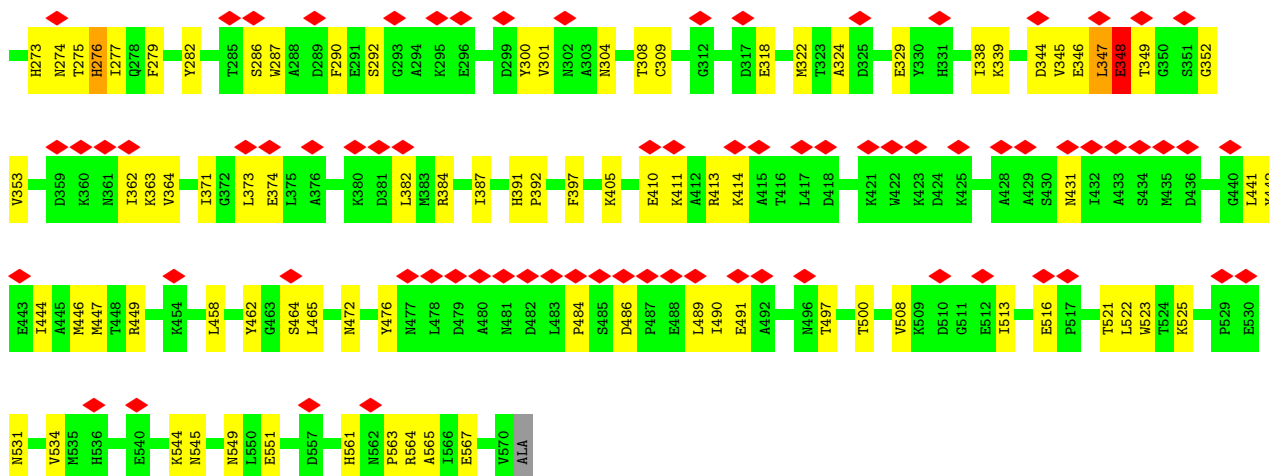
Chain L: 37% 14% 46%



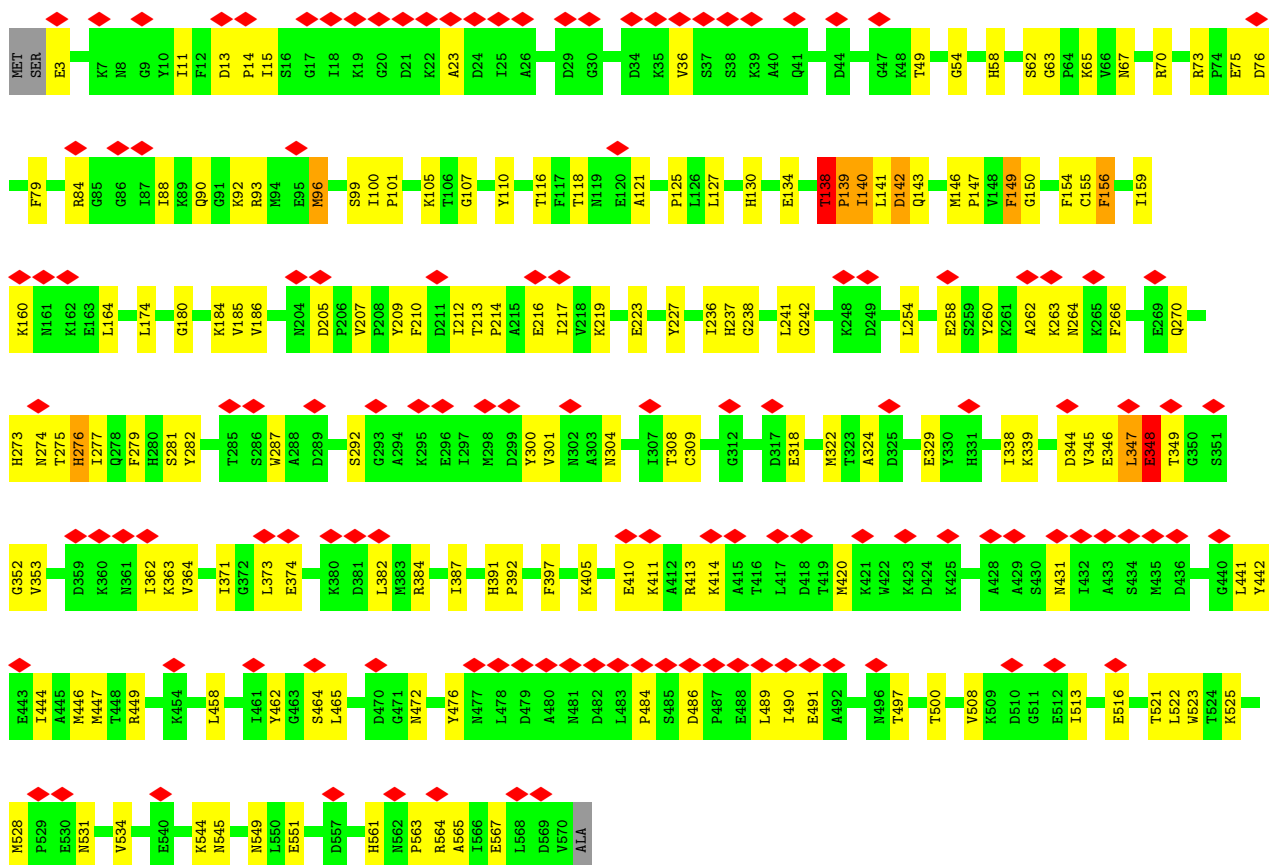
- Molecule 9: Formylmethanofuran dehydrogenase, subunit A

Chain G: 22% 70% 27%



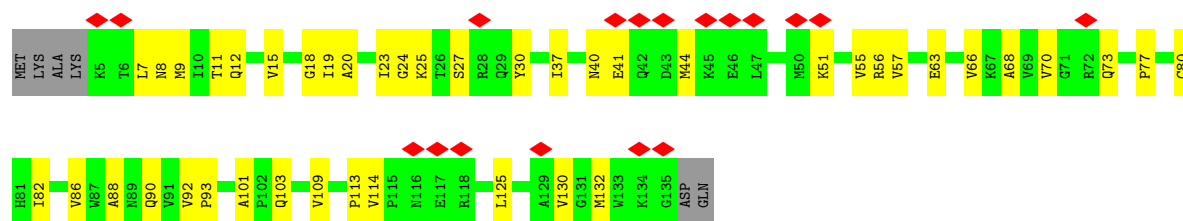


• Molecule 9: Formylmethanofuran dehydrogenase, subunit A

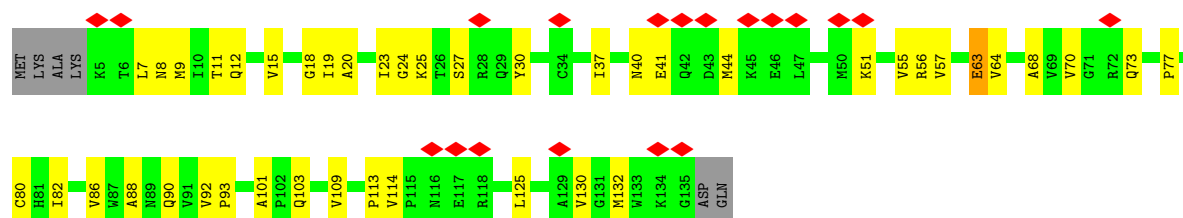


• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

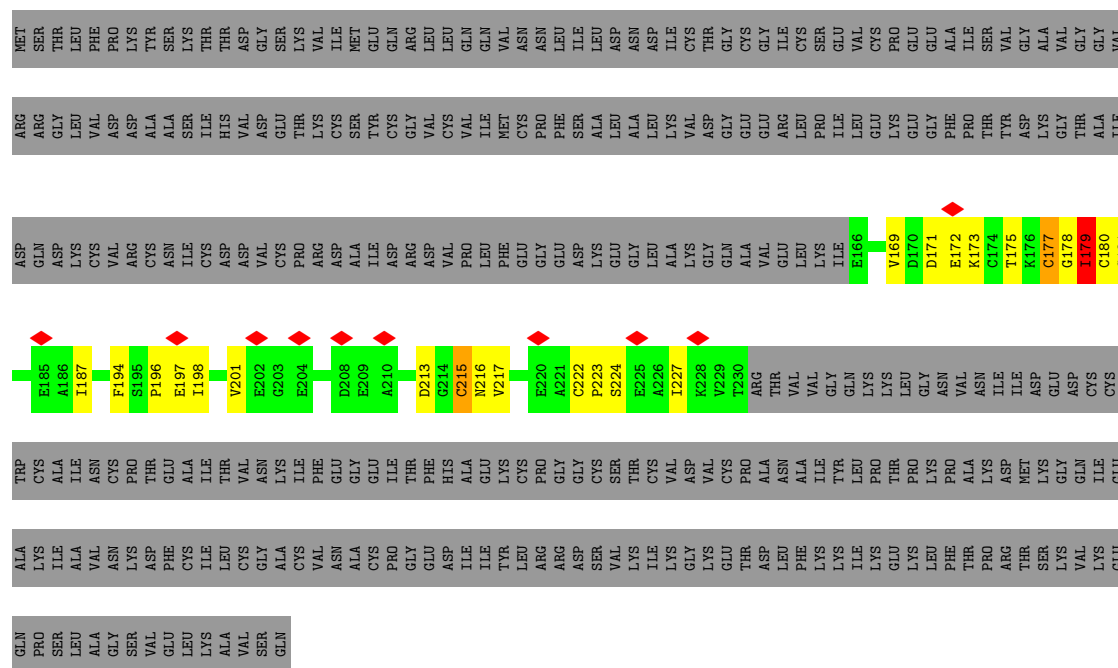




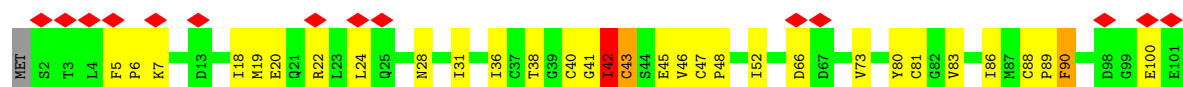
- Molecule 10: Formylmethanofuran dehydrogenase, subunit D



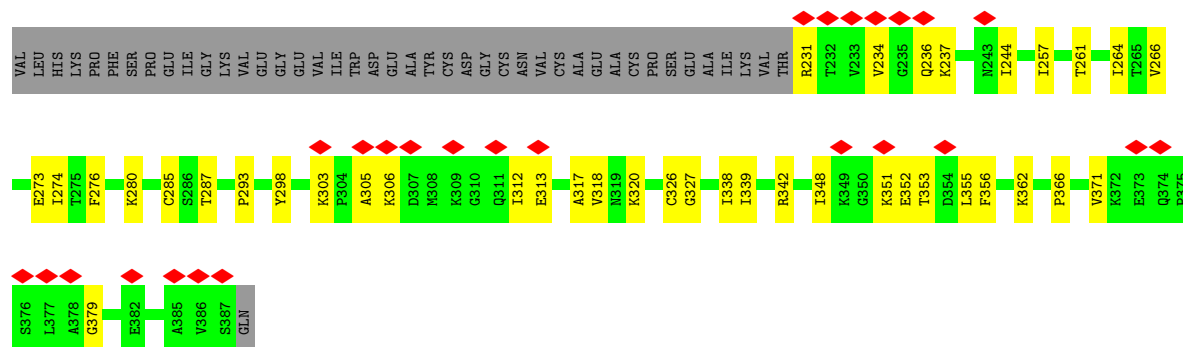
- Molecule 11: Formylmethanofuran dehydrogenase, subunit F



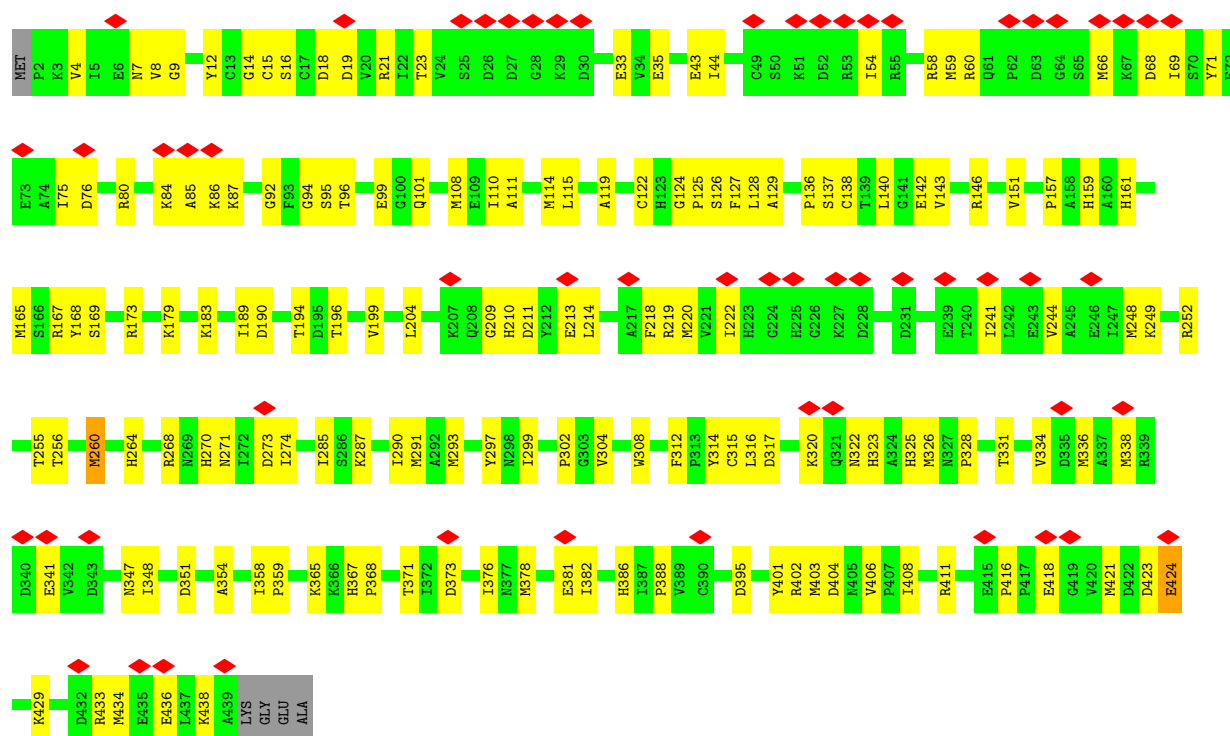
- Molecule 11: Formylmethanofuran dehydrogenase, subunit F



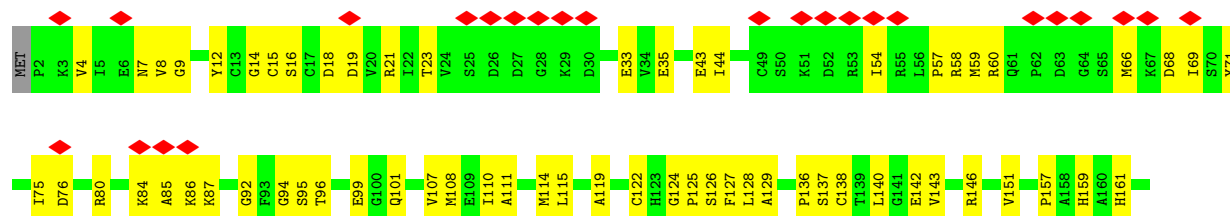


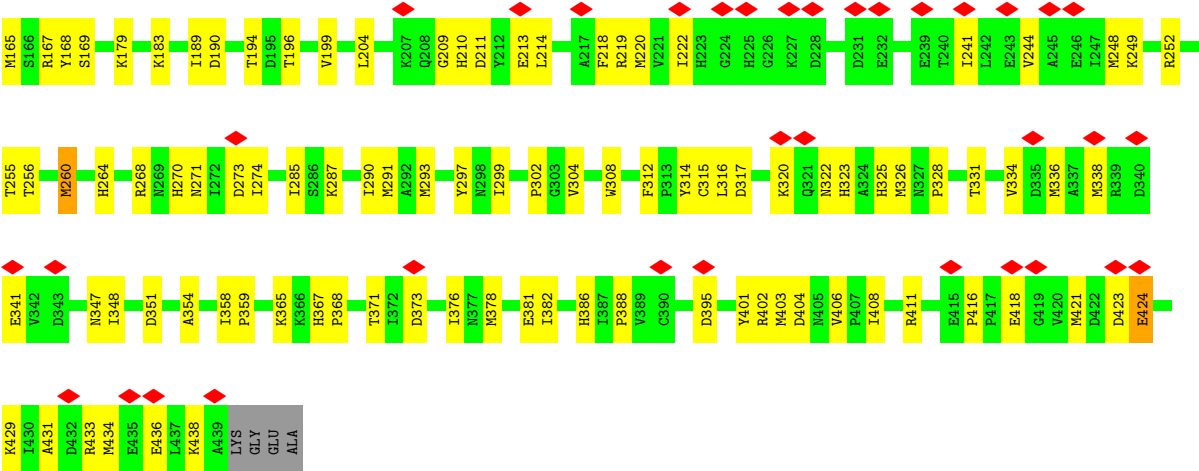


• Molecule 12: Formylmethanofuran dehydrogenase, subunit B



• Molecule 12: Formylmethanofuran dehydrogenase, subunit B





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 1239454                                 | 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 ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 103.221                                 | Depositor |
| Minimum map value                    | -64.149                                 | Depositor |
| Average map value                    | -0.069                                  | Depositor |
| Map value standard deviation         | 1.898                                   | Depositor |
| Recommended contour level            | 10                                      | Depositor |
| Map size (Å)                         | 361.584, 361.584, 361.584               | wwPDB     |
| Map dimensions                       | 432, 432, 432                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.837, 0.837, 0.837                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, MO, KCX, MGD, SF4, 9S8, FAD, ZN

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     | 0.46         | 0/5115      | 0.64        | 3/6920 (0.0%)   |
| 1   | a     | 0.47         | 0/5115      | 0.65        | 2/6920 (0.0%)   |
| 2   | F     | 0.49         | 0/1096      | 0.64        | 1/1474 (0.1%)   |
| 2   | f     | 0.49         | 0/1096      | 0.64        | 1/1474 (0.1%)   |
| 3   | E     | 0.59         | 0/3208      | 0.74        | 1/4314 (0.0%)   |
| 3   | e     | 0.59         | 0/3208      | 0.74        | 1/4314 (0.0%)   |
| 4   | C     | 0.31         | 0/1529      | 0.41        | 0/2072          |
| 4   | c     | 0.31         | 0/1529      | 0.41        | 0/2072          |
| 5   | B     | 0.43         | 0/2355      | 0.62        | 2/3187 (0.1%)   |
| 5   | b     | 0.43         | 0/2355      | 0.62        | 2/3187 (0.1%)   |
| 6   | D     | 0.49         | 0/4345      | 0.70        | 7/5889 (0.1%)   |
| 6   | d     | 0.50         | 0/4345      | 0.70        | 7/5889 (0.1%)   |
| 7   | I     | 0.47         | 0/2029      | 0.73        | 1/2724 (0.0%)   |
| 7   | i     | 0.47         | 0/2029      | 0.73        | 1/2724 (0.0%)   |
| 8   | L     | 0.80         | 0/585       | 1.12        | 3/800 (0.4%)    |
| 8   | l     | 0.80         | 0/585       | 1.12        | 3/800 (0.4%)    |
| 9   | G     | 0.42         | 0/4549      | 0.65        | 10/6174 (0.2%)  |
| 9   | g     | 0.42         | 0/4549      | 0.65        | 10/6174 (0.2%)  |
| 10  | J     | 0.36         | 0/1023      | 0.57        | 0/1383          |
| 10  | j     | 0.36         | 0/1023      | 0.57        | 0/1383          |
| 11  | K     | 0.65         | 0/2455      | 0.88        | 4/3313 (0.1%)   |
| 11  | M     | 0.67         | 0/495       | 1.17        | 2/669 (0.3%)    |
| 11  | k     | 0.66         | 0/2455      | 0.88        | 4/3313 (0.1%)   |
| 11  | m     | 0.67         | 0/495       | 1.17        | 2/669 (0.3%)    |
| 12  | H     | 0.51         | 0/3497      | 0.68        | 1/4732 (0.0%)   |
| 12  | h     | 0.51         | 0/3497      | 0.68        | 1/4732 (0.0%)   |
| All | All   | 0.50         | 0/64562     | 0.70        | 69/87302 (0.1%) |

There are no bond length outliers.

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | F     | 96  | ILE  | N-CA-C  | -8.36 | 104.56      | 112.83   |
| 2   | f     | 96  | ILE  | N-CA-C  | -8.35 | 104.56      | 112.83   |
| 11  | k     | 128 | CYS  | N-CA-C  | 8.14  | 120.23      | 111.36   |
| 11  | K     | 128 | CYS  | N-CA-C  | 8.13  | 120.22      | 111.36   |
| 7   | I     | 12  | PRO  | CB-CA-C | -7.77 | 102.02      | 111.11   |
| 7   | i     | 12  | PRO  | CB-CA-C | -7.76 | 102.03      | 111.11   |
| 9   | g     | 156 | PHE  | N-CA-C  | -7.44 | 103.83      | 113.12   |
| 9   | G     | 156 | PHE  | N-CA-C  | -7.43 | 103.83      | 113.12   |
| 9   | g     | 139 | PRO  | N-CA-C  | 7.40  | 127.71      | 112.47   |
| 9   | G     | 139 | PRO  | N-CA-C  | 7.39  | 127.70      | 112.47   |
| 3   | e     | 307 | TYR  | CB-CA-C | -7.25 | 99.27       | 111.02   |
| 3   | E     | 307 | TYR  | CB-CA-C | -7.23 | 99.31       | 111.02   |
| 8   | l     | 131 | TYR  | CB-CA-C | -7.04 | 99.92       | 111.68   |
| 11  | k     | 128 | CYS  | CA-C-O  | -7.04 | 112.96      | 120.42   |
| 8   | L     | 131 | TYR  | CB-CA-C | -7.03 | 99.94       | 111.68   |
| 11  | K     | 128 | CYS  | CA-C-O  | -7.02 | 112.97      | 120.42   |
| 11  | k     | 43  | CYS  | N-CA-C  | -6.90 | 105.41      | 114.31   |
| 11  | K     | 43  | CYS  | N-CA-C  | -6.89 | 105.42      | 114.31   |
| 8   | L     | 79  | CYS  | N-CA-C  | -6.67 | 105.27      | 113.41   |
| 8   | l     | 79  | CYS  | N-CA-C  | -6.67 | 105.28      | 113.41   |
| 1   | A     | 651 | GLN  | N-CA-C  | 6.58  | 118.45      | 111.28   |
| 1   | a     | 651 | GLN  | N-CA-C  | 6.56  | 118.43      | 111.28   |
| 9   | G     | 149 | PHE  | CB-CA-C | -6.37 | 100.70      | 111.02   |
| 9   | g     | 149 | PHE  | CB-CA-C | -6.36 | 100.72      | 111.02   |
| 9   | g     | 142 | ASP  | N-CA-C  | -6.12 | 102.28      | 110.55   |
| 9   | G     | 142 | ASP  | N-CA-C  | -6.12 | 102.29      | 110.55   |
| 11  | k     | 80  | TYR  | CB-CA-C | 6.05  | 120.32      | 111.73   |
| 11  | K     | 80  | TYR  | CB-CA-C | 6.04  | 120.31      | 111.73   |
| 6   | d     | 530 | PRO  | N-CA-C  | 6.00  | 121.36      | 113.86   |
| 6   | D     | 530 | PRO  | N-CA-C  | 5.96  | 121.31      | 113.86   |
| 5   | B     | 193 | ASN  | CB-CA-C | 5.86  | 120.21      | 111.89   |
| 5   | b     | 193 | ASN  | CB-CA-C | 5.86  | 120.20      | 111.89   |
| 6   | d     | 37  | GLU  | CB-CA-C | 5.75  | 117.52      | 108.84   |
| 6   | D     | 37  | GLU  | CB-CA-C | 5.74  | 117.50      | 108.84   |
| 6   | d     | 45  | ASN  | CA-C-N  | -5.69 | 113.54      | 122.08   |
| 6   | d     | 45  | ASN  | C-N-CA  | -5.69 | 113.54      | 122.08   |
| 6   | D     | 45  | ASN  | CA-C-N  | -5.67 | 113.58      | 122.08   |
| 6   | D     | 45  | ASN  | C-N-CA  | -5.67 | 113.58      | 122.08   |
| 1   | A     | 193 | PHE  | CA-C-O  | -5.62 | 114.69      | 120.87   |
| 9   | g     | 138 | THR  | CB-CA-C | 5.55  | 118.34      | 109.62   |
| 9   | G     | 138 | THR  | CB-CA-C | 5.54  | 118.32      | 109.62   |
| 6   | D     | 45  | ASN  | N-CA-C  | -5.52 | 99.43       | 108.76   |
| 6   | d     | 45  | ASN  | N-CA-C  | -5.52 | 99.44       | 108.76   |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | d     | 46  | GLU  | CB-CA-C  | 5.51  | 119.65      | 111.88   |
| 6   | D     | 46  | GLU  | CB-CA-C  | 5.50  | 119.64      | 111.88   |
| 9   | G     | 154 | PHE  | CA-CB-CG | 5.50  | 119.30      | 113.80   |
| 9   | g     | 154 | PHE  | CA-CB-CG | 5.45  | 119.25      | 113.80   |
| 8   | L     | 85  | VAL  | N-CA-C   | -5.32 | 105.94      | 111.58   |
| 11  | M     | 213 | ASP  | N-CA-C   | -5.32 | 100.38      | 107.88   |
| 8   | l     | 85  | VAL  | N-CA-C   | -5.31 | 105.95      | 111.58   |
| 1   | a     | 406 | ARG  | N-CA-C   | -5.30 | 104.33      | 111.54   |
| 1   | A     | 406 | ARG  | N-CA-C   | -5.30 | 104.33      | 111.54   |
| 12  | H     | 127 | PHE  | N-CA-C   | -5.28 | 105.52      | 111.28   |
| 11  | m     | 213 | ASP  | N-CA-C   | -5.27 | 100.45      | 107.88   |
| 9   | G     | 139 | PRO  | CB-CA-C  | -5.26 | 102.88      | 111.56   |
| 9   | g     | 139 | PRO  | CB-CA-C  | -5.26 | 102.88      | 111.56   |
| 12  | h     | 127 | PHE  | N-CA-C   | -5.25 | 105.56      | 111.28   |
| 6   | d     | 526 | CYS  | CB-CA-C  | 5.24  | 119.11      | 109.46   |
| 6   | D     | 526 | CYS  | CB-CA-C  | 5.23  | 119.08      | 109.46   |
| 9   | g     | 347 | LEU  | CA-C-O   | -5.18 | 115.58      | 121.65   |
| 9   | G     | 347 | LEU  | CA-C-O   | -5.16 | 115.61      | 121.65   |
| 11  | M     | 223 | PRO  | N-CA-C   | -5.15 | 106.11      | 113.47   |
| 11  | m     | 223 | PRO  | N-CA-C   | -5.15 | 106.11      | 113.47   |
| 9   | g     | 348 | GLU  | CA-C-N   | -5.10 | 114.68      | 122.23   |
| 9   | g     | 348 | GLU  | C-N-CA   | -5.10 | 114.68      | 122.23   |
| 9   | G     | 348 | GLU  | CA-C-N   | -5.09 | 114.69      | 122.23   |
| 9   | G     | 348 | GLU  | C-N-CA   | -5.09 | 114.69      | 122.23   |
| 5   | B     | 153 | ALA  | N-CA-C   | 5.07  | 117.87      | 109.46   |
| 5   | b     | 153 | ALA  | N-CA-C   | 5.06  | 117.86      | 109.46   |

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     | 5011  | 0        | 4967     | 71      | 0            |
| 1   | a     | 5011  | 0        | 4967     | 70      | 0            |
| 2   | F     | 1073  | 0        | 1082     | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | f     | 1073  | 0        | 1082     | 25      | 0            |
| 3   | E     | 3151  | 0        | 3162     | 52      | 0            |
| 3   | e     | 3151  | 0        | 3162     | 51      | 0            |
| 4   | C     | 1498  | 0        | 1495     | 27      | 0            |
| 4   | c     | 1498  | 0        | 1495     | 26      | 0            |
| 5   | B     | 2304  | 0        | 2272     | 42      | 0            |
| 5   | b     | 2304  | 0        | 2272     | 44      | 0            |
| 6   | D     | 4251  | 0        | 4204     | 95      | 0            |
| 6   | d     | 4251  | 0        | 4204     | 101     | 0            |
| 7   | I     | 1996  | 0        | 2001     | 54      | 0            |
| 7   | i     | 1996  | 0        | 2001     | 61      | 0            |
| 8   | L     | 576   | 0        | 559      | 18      | 0            |
| 8   | l     | 576   | 0        | 559      | 15      | 0            |
| 9   | G     | 4455  | 0        | 4380     | 125     | 0            |
| 9   | g     | 4455  | 0        | 4380     | 127     | 0            |
| 10  | J     | 1007  | 0        | 1022     | 37      | 0            |
| 10  | j     | 1007  | 0        | 1022     | 39      | 0            |
| 11  | K     | 2423  | 0        | 2435     | 57      | 0            |
| 11  | M     | 487   | 0        | 457      | 9       | 0            |
| 11  | k     | 2423  | 0        | 2435     | 59      | 0            |
| 11  | m     | 487   | 0        | 457      | 10      | 0            |
| 12  | H     | 3416  | 0        | 3354     | 108     | 0            |
| 12  | h     | 3416  | 0        | 3354     | 110     | 0            |
| 13  | A     | 48    | 0        | 0        | 2       | 0            |
| 13  | C     | 16    | 0        | 0        | 1       | 0            |
| 13  | D     | 8     | 0        | 0        | 0       | 0            |
| 13  | E     | 32    | 0        | 0        | 0       | 0            |
| 13  | H     | 8     | 0        | 0        | 0       | 0            |
| 13  | K     | 48    | 0        | 0        | 1       | 0            |
| 13  | L     | 16    | 0        | 0        | 0       | 0            |
| 13  | M     | 16    | 0        | 0        | 0       | 0            |
| 13  | a     | 48    | 0        | 0        | 2       | 0            |
| 13  | c     | 16    | 0        | 0        | 1       | 0            |
| 13  | d     | 8     | 0        | 0        | 0       | 0            |
| 13  | e     | 32    | 0        | 0        | 0       | 0            |
| 13  | h     | 8     | 0        | 0        | 0       | 0            |
| 13  | k     | 48    | 0        | 0        | 1       | 0            |
| 13  | l     | 16    | 0        | 0        | 0       | 0            |
| 13  | m     | 16    | 0        | 0        | 0       | 0            |
| 14  | A     | 53    | 0        | 31       | 0       | 0            |
| 14  | E     | 53    | 0        | 31       | 1       | 0            |
| 14  | a     | 53    | 0        | 31       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | e     | 53    | 0        | 31       | 0       | 0            |
| 15  | F     | 4     | 0        | 0        | 0       | 0            |
| 15  | f     | 4     | 0        | 0        | 0       | 0            |
| 16  | B     | 16    | 0        | 0        | 1       | 0            |
| 16  | b     | 16    | 0        | 0        | 1       | 0            |
| 17  | G     | 2     | 0        | 0        | 0       | 0            |
| 17  | g     | 2     | 0        | 0        | 0       | 0            |
| 18  | H     | 1     | 0        | 0        | 0       | 0            |
| 18  | h     | 1     | 0        | 0        | 0       | 0            |
| 19  | H     | 94    | 0        | 44       | 8       | 0            |
| 19  | h     | 94    | 0        | 44       | 8       | 0            |
| All | All   | 64126 | 0        | 62992    | 1323    | 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 10.

All (1323) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 9:G:107:GLY:HA3  | 9:G:139:PRO:HD2   | 1.49                     | 0.92              |
| 9:g:107:GLY:HA3  | 9:g:139:PRO:HD2   | 1.49                     | 0.92              |
| 10:j:11:THR:HG21 | 19:h:503:MGD:H191 | 1.34                     | 0.92              |
| 10:J:11:THR:HG21 | 19:H:503:MGD:H191 | 1.34                     | 0.92              |
| 7:i:74:ARG:HG3   | 7:i:93:ASP:HB2    | 1.58                     | 0.85              |
| 7:I:74:ARG:HG3   | 7:I:93:ASP:HB2    | 1.58                     | 0.83              |
| 5:b:53:ASP:HB3   | 5:b:56:VAL:HG12   | 1.65                     | 0.79              |
| 4:C:125:PHE:HB3  | 5:B:52:ILE:HD11   | 1.65                     | 0.79              |
| 4:c:125:PHE:HB3  | 5:b:52:ILE:HD11   | 1.65                     | 0.79              |
| 9:G:186:VAL:HG11 | 9:G:324:ALA:HB3   | 1.65                     | 0.78              |
| 9:G:15:ILE:HD12  | 9:G:464:SER:HB2   | 1.66                     | 0.78              |
| 5:B:53:ASP:HB3   | 5:B:56:VAL:HG12   | 1.65                     | 0.77              |
| 9:g:186:VAL:HG11 | 9:g:324:ALA:HB3   | 1.65                     | 0.77              |
| 9:g:15:ILE:HD12  | 9:g:464:SER:HB2   | 1.66                     | 0.77              |
| 9:G:125:PRO:HD2  | 9:G:348:GLU:HG2   | 1.67                     | 0.77              |
| 9:g:125:PRO:HD2  | 9:g:348:GLU:HG2   | 1.67                     | 0.76              |
| 9:G:387:ILE:HG13 | 9:G:447:MET:HE2   | 1.69                     | 0.75              |
| 3:e:48:LYS:HG2   | 3:e:73:LEU:HD21   | 1.66                     | 0.75              |
| 3:E:48:LYS:HG2   | 3:E:73:LEU:HD21   | 1.66                     | 0.75              |
| 9:g:387:ILE:HG13 | 9:g:447:MET:HE2   | 1.69                     | 0.75              |
| 9:G:258:GLU:OE2  | 9:G:304:ASN:ND2   | 2.20                     | 0.74              |
| 3:e:79:LEU:HD21  | 3:e:304:PRO:HG3   | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:129:PHE:HD2  | 6:D:131:THR:HG23 | 1.54                     | 0.73              |
| 6:d:129:PHE:HD2  | 6:d:131:THR:HG23 | 1.53                     | 0.72              |
| 9:g:258:GLU:OE2  | 9:g:304:ASN:ND2  | 2.20                     | 0.72              |
| 3:E:79:LEU:HD21  | 3:E:304:PRO:HG3  | 1.69                     | 0.72              |
| 2:f:15:ASN:OD1   | 2:f:40:ARG:NH1   | 2.23                     | 0.72              |
| 7:I:253:LYS:HG3  | 7:I:254:LYS:H    | 1.54                     | 0.72              |
| 11:k:161:VAL:HA  | 11:k:237:LYS:HG2 | 1.71                     | 0.72              |
| 3:e:368:GLU:HA   | 3:e:371:LYS:HG2  | 1.72                     | 0.72              |
| 4:C:76:GLU:OE2   | 4:C:118:ARG:NH2  | 2.23                     | 0.71              |
| 7:i:229:GLU:HB2  | 7:i:236:THR:HG23 | 1.72                     | 0.71              |
| 10:j:20:ALA:HB1  | 10:j:30:TYR:HA   | 1.72                     | 0.71              |
| 4:c:76:GLU:OE2   | 4:c:118:ARG:NH2  | 2.23                     | 0.71              |
| 3:E:152:THR:HG22 | 3:E:167:TYR:HB2  | 1.73                     | 0.71              |
| 2:F:15:ASN:OD1   | 2:F:40:ARG:NH1   | 2.23                     | 0.71              |
| 11:K:161:VAL:HA  | 11:K:237:LYS:HG2 | 1.71                     | 0.71              |
| 9:G:185:VAL:HB   | 9:G:236:ILE:HD12 | 1.73                     | 0.71              |
| 10:j:73:GLN:HE21 | 12:h:194:THR:HA  | 1.55                     | 0.71              |
| 10:J:73:GLN:HE21 | 12:H:194:THR:HA  | 1.55                     | 0.71              |
| 2:f:82:ALA:O     | 2:f:86:MET:HG2   | 1.91                     | 0.71              |
| 7:i:253:LYS:HG3  | 7:i:254:LYS:H    | 1.54                     | 0.71              |
| 9:g:185:VAL:HB   | 9:g:236:ILE:HD12 | 1.73                     | 0.71              |
| 12:h:59:MET:HE3  | 12:h:69:ILE:HD13 | 1.73                     | 0.70              |
| 2:F:82:ALA:O     | 2:F:86:MET:HG2   | 1.91                     | 0.70              |
| 3:E:368:GLU:HA   | 3:E:371:LYS:HG2  | 1.72                     | 0.70              |
| 7:I:229:GLU:HB2  | 7:I:236:THR:HG23 | 1.72                     | 0.70              |
| 1:A:96:ARG:NH1   | 1:A:138:ASP:OD1  | 2.23                     | 0.70              |
| 6:D:351:SER:O    | 6:D:354:GLN:NE2  | 2.22                     | 0.70              |
| 3:e:152:THR:HG22 | 3:e:167:TYR:HB2  | 1.73                     | 0.70              |
| 12:H:59:MET:HE3  | 12:H:69:ILE:HD13 | 1.73                     | 0.70              |
| 7:I:144:TRP:HH2  | 9:G:73:ARG:HH12  | 1.39                     | 0.70              |
| 9:G:54:GLY:HA2   | 9:G:449:ARG:HG3  | 1.72                     | 0.70              |
| 6:d:364:LYS:NZ   | 6:d:507:VAL:O    | 2.25                     | 0.70              |
| 12:H:354:ALA:HB2 | 12:H:378:MET:HG3 | 1.73                     | 0.70              |
| 10:J:20:ALA:HB1  | 10:J:30:TYR:HA   | 1.72                     | 0.69              |
| 1:a:96:ARG:NH1   | 1:a:138:ASP:OD1  | 2.23                     | 0.69              |
| 1:A:575:SER:HB2  | 1:a:575:SER:HB2  | 1.74                     | 0.69              |
| 1:a:211:GLY:HA3  | 1:a:297:MET:HE2  | 1.75                     | 0.69              |
| 9:G:301:VAL:O    | 9:G:384:ARG:NH2  | 2.26                     | 0.69              |
| 7:I:248:GLU:OE1  | 12:H:219:ARG:NH2 | 2.25                     | 0.69              |
| 7:i:248:GLU:OE1  | 12:h:219:ARG:NH2 | 2.25                     | 0.69              |
| 9:g:67:ASN:OD1   | 9:g:130:HIS:NE2  | 2.24                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:364:LYS:NZ    | 6:D:507:VAL:O     | 2.25                     | 0.69              |
| 12:H:114:MET:HG3  | 12:H:336:MET:HE1  | 1.74                     | 0.69              |
| 3:e:162:GLN:HB3   | 3:e:175:LYS:HE2   | 1.75                     | 0.69              |
| 9:g:54:GLY:HA2    | 9:g:449:ARG:HG3   | 1.73                     | 0.69              |
| 12:h:114:MET:HG3  | 12:h:336:MET:HE1  | 1.74                     | 0.69              |
| 9:g:301:VAL:O     | 9:g:384:ARG:NH2   | 2.26                     | 0.69              |
| 10:j:11:THR:HG21  | 19:h:503:MGD:N19  | 2.07                     | 0.68              |
| 7:i:144:TRP:HH2   | 9:g:73:ARG:HH12   | 1.39                     | 0.68              |
| 1:A:211:GLY:HA3   | 1:A:297:MET:HE2   | 1.75                     | 0.68              |
| 7:i:23:PRO:HD2    | 7:i:83:MET:HG3    | 1.75                     | 0.68              |
| 12:h:354:ALA:HB2  | 12:h:378:MET:HG3  | 1.73                     | 0.68              |
| 9:g:344:ASP:OD1   | 12:h:287:LYS:NZ   | 2.27                     | 0.68              |
| 7:I:23:PRO:HD2    | 7:I:83:MET:HG3    | 1.75                     | 0.67              |
| 11:k:7:LYS:HB2    | 11:k:22:ARG:HB2   | 1.75                     | 0.67              |
| 9:G:449:ARG:NH2   | 9:G:476:TYR:OH    | 2.27                     | 0.67              |
| 12:h:19:ASP:OD2   | 12:h:167:ARG:NH1  | 2.23                     | 0.67              |
| 9:G:344:ASP:OD1   | 12:H:287:LYS:NZ   | 2.27                     | 0.67              |
| 9:g:549:ASN:ND2   | 12:h:7:ASN:OD1    | 2.26                     | 0.67              |
| 1:A:387:ARG:HD2   | 1:A:503:ASP:HB3   | 1.77                     | 0.67              |
| 3:E:162:GLN:HB3   | 3:E:175:LYS:HE2   | 1.75                     | 0.67              |
| 1:a:387:ARG:HD2   | 1:a:503:ASP:HB3   | 1.77                     | 0.67              |
| 9:g:449:ARG:NH2   | 9:g:476:TYR:OH    | 2.27                     | 0.67              |
| 10:J:11:THR:HG21  | 19:H:503:MGD:N19  | 2.07                     | 0.66              |
| 12:H:60:ARG:NH2   | 12:H:381:GLU:O    | 2.29                     | 0.66              |
| 6:d:351:SER:O     | 6:d:354:GLN:NE2   | 2.22                     | 0.66              |
| 9:g:65:LYS:HZ1    | 9:g:324:ALA:HB2   | 1.61                     | 0.66              |
| 11:K:7:LYS:HB2    | 11:K:22:ARG:HB2   | 1.75                     | 0.66              |
| 9:G:67:ASN:OD1    | 9:G:130:HIS:NE2   | 2.24                     | 0.66              |
| 9:G:549:ASN:ND2   | 12:H:7:ASN:OD1    | 2.26                     | 0.66              |
| 1:A:431:ILE:HD11  | 1:A:440:ALA:HB2   | 1.76                     | 0.66              |
| 1:a:431:ILE:HD11  | 1:a:440:ALA:HB2   | 1.76                     | 0.66              |
| 11:K:163:LEU:HD21 | 11:K:231:ARG:HH21 | 1.61                     | 0.65              |
| 3:E:152:THR:HG23  | 3:E:168:GLU:HG3   | 1.78                     | 0.65              |
| 6:D:236:ILE:HD11  | 6:D:317:LEU:HD11  | 1.78                     | 0.65              |
| 6:d:122:GLN:OE1   | 6:d:126:ARG:NH1   | 2.30                     | 0.65              |
| 2:F:112:GLU:HB3   | 2:F:115:LYS:HB3   | 1.78                     | 0.65              |
| 12:h:60:ARG:NH2   | 12:h:381:GLU:O    | 2.29                     | 0.65              |
| 6:d:236:ILE:HD11  | 6:d:317:LEU:HD11  | 1.78                     | 0.64              |
| 9:g:486:ASP:HB3   | 9:g:489:LEU:HD23  | 1.79                     | 0.64              |
| 11:k:163:LEU:HD21 | 11:k:231:ARG:HH21 | 1.61                     | 0.64              |
| 9:G:405:LYS:HD3   | 9:G:491:GLU:HG3   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:e:152:THR:HG23  | 3:e:168:GLU:HG3  | 1.78                     | 0.64              |
| 12:H:260:MET:HE3  | 12:H:264:HIS:CE1 | 2.33                     | 0.64              |
| 12:H:19:ASP:OD2   | 12:H:167:ARG:NH1 | 2.23                     | 0.64              |
| 2:f:112:GLU:HB3   | 2:f:115:LYS:HB3  | 1.78                     | 0.64              |
| 12:h:137:SER:OG   | 12:h:138:CYS:N   | 2.31                     | 0.64              |
| 9:G:523:TRP:HE1   | 9:G:563:PRO:HB2  | 1.63                     | 0.63              |
| 3:E:123:ILE:HG12  | 3:E:227:LYS:HD3  | 1.80                     | 0.63              |
| 6:D:170:LEU:HD23  | 6:D:284:TYR:HA   | 1.81                     | 0.63              |
| 9:G:287:TRP:O     | 9:G:363:LYS:NZ   | 2.31                     | 0.63              |
| 9:g:405:LYS:HD3   | 9:g:491:GLU:HG3  | 1.79                     | 0.63              |
| 9:G:486:ASP:HB3   | 9:G:489:LEU:HD23 | 1.79                     | 0.63              |
| 9:g:523:TRP:HE1   | 9:g:563:PRO:HB2  | 1.63                     | 0.63              |
| 6:D:140:ILE:HD13  | 6:D:407:TYR:HE2  | 1.63                     | 0.62              |
| 11:K:312:ILE:HG23 | 11:K:313:GLU:H   | 1.64                     | 0.62              |
| 3:e:123:ILE:HG12  | 3:e:227:LYS:HD3  | 1.80                     | 0.62              |
| 9:g:110:TYR:HB3   | 9:g:141:LEU:HD21 | 1.81                     | 0.62              |
| 12:H:137:SER:OG   | 12:H:138:CYS:N   | 2.31                     | 0.62              |
| 6:d:170:LEU:HD23  | 6:d:284:TYR:HA   | 1.81                     | 0.62              |
| 12:h:260:MET:HE3  | 12:h:264:HIS:CE1 | 2.33                     | 0.62              |
| 6:D:174:TRP:CG    | 6:D:311:MET:HE1  | 2.35                     | 0.62              |
| 6:d:140:ILE:HD13  | 6:d:407:TYR:HE2  | 1.63                     | 0.62              |
| 6:D:122:GLN:OE1   | 6:D:126:ARG:NH1  | 2.30                     | 0.62              |
| 9:G:110:TYR:HB2   | 9:G:141:LEU:HD11 | 1.81                     | 0.62              |
| 9:G:110:TYR:HB3   | 9:G:141:LEU:HD21 | 1.81                     | 0.62              |
| 10:J:19:ILE:HG23  | 12:H:43:GLU:OE1  | 1.99                     | 0.62              |
| 9:G:264:ASN:ND2   | 9:G:266:PHE:O    | 2.33                     | 0.62              |
| 1:a:161:GLN:HG2   | 1:a:567:VAL:HG13 | 1.82                     | 0.62              |
| 10:j:19:ILE:HG23  | 12:h:43:GLU:OE1  | 1.99                     | 0.62              |
| 11:K:38:THR:HB    | 11:K:293:PRO:HG3 | 1.82                     | 0.62              |
| 2:f:13:ILE:HG22   | 2:f:66:SER:HB3   | 1.82                     | 0.62              |
| 3:E:118:ASN:ND2   | 3:E:121:ASN:OD1  | 2.33                     | 0.61              |
| 11:M:196:PRO:HG2  | 11:K:298:TYR:HB3 | 1.83                     | 0.61              |
| 3:e:118:ASN:ND2   | 3:e:121:ASN:OD1  | 2.33                     | 0.61              |
| 6:d:174:TRP:CG    | 6:d:311:MET:HE1  | 2.35                     | 0.61              |
| 11:k:312:ILE:HG23 | 11:k:313:GLU:H   | 1.64                     | 0.61              |
| 2:F:13:ILE:HG22   | 2:F:66:SER:HB3   | 1.82                     | 0.61              |
| 9:G:274:ASN:HD22  | 9:G:277:ILE:HG12 | 1.66                     | 0.61              |
| 5:b:66:VAL:HG23   | 5:b:112:MET:HE2  | 1.83                     | 0.61              |
| 9:g:110:TYR:HB2   | 9:g:141:LEU:HD11 | 1.81                     | 0.61              |
| 11:k:38:THR:HB    | 11:k:293:PRO:HG3 | 1.82                     | 0.61              |
| 9:g:264:ASN:ND2   | 9:g:266:PHE:O    | 2.33                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:41:GLY:C    | 11:K:43:CYS:H     | 2.08                     | 0.61              |
| 6:d:235:ILE:HG12 | 6:d:285:ALA:HB2   | 1.83                     | 0.61              |
| 11:k:41:GLY:C    | 11:k:43:CYS:H     | 2.08                     | 0.61              |
| 4:C:55:PRO:O     | 4:C:59:ARG:NH1    | 2.34                     | 0.61              |
| 1:A:161:GLN:HG2  | 1:A:567:VAL:HG13  | 1.82                     | 0.61              |
| 2:F:61:ASP:OD1   | 2:F:136:LYS:NZ    | 2.34                     | 0.61              |
| 5:B:233:GLU:HG2  | 5:B:235:CYS:H     | 1.66                     | 0.61              |
| 6:D:235:ILE:HG12 | 6:D:285:ALA:HB2   | 1.83                     | 0.61              |
| 6:D:310:SER:HA   | 6:D:313:ASN:HD22  | 1.66                     | 0.61              |
| 9:g:274:ASN:HD22 | 9:g:277:ILE:HG12  | 1.66                     | 0.60              |
| 9:g:329:GLU:HG3  | 9:g:352:GLY:HA3   | 1.83                     | 0.60              |
| 1:A:429:HIS:HB2  | 1:A:461:ILE:HD12  | 1.82                     | 0.60              |
| 3:E:177:ASP:OD2  | 3:E:178:GLU:N     | 2.35                     | 0.60              |
| 4:C:61:SER:OG    | 4:C:84:ASP:OD2    | 2.20                     | 0.60              |
| 9:G:329:GLU:HG3  | 9:G:352:GLY:HA3   | 1.83                     | 0.60              |
| 9:g:237:HIS:CD2  | 9:g:276:HIS:CE1   | 2.90                     | 0.60              |
| 11:m:196:PRO:HG2 | 11:k:298:TYR:HB3  | 1.83                     | 0.60              |
| 9:G:237:HIS:CD2  | 9:G:276:HIS:CE1   | 2.90                     | 0.60              |
| 4:c:55:PRO:O     | 4:c:59:ARG:NH1    | 2.34                     | 0.60              |
| 5:B:66:VAL:HG23  | 5:B:112:MET:HE2   | 1.83                     | 0.60              |
| 9:G:127:LEU:HD21 | 12:H:406:VAL:HG22 | 1.83                     | 0.60              |
| 1:a:429:HIS:HB2  | 1:a:461:ILE:HD12  | 1.82                     | 0.60              |
| 9:g:287:TRP:O    | 9:g:363:LYS:NZ    | 2.31                     | 0.60              |
| 3:e:177:ASP:OD2  | 3:e:178:GLU:N     | 2.35                     | 0.60              |
| 7:I:176:ASP:HB2  | 7:I:195:ASP:O     | 2.02                     | 0.60              |
| 7:i:176:ASP:HB2  | 7:i:195:ASP:O     | 2.02                     | 0.60              |
| 9:g:186:VAL:HG13 | 9:g:237:HIS:ND1   | 2.16                     | 0.60              |
| 5:b:233:GLU:HG2  | 5:b:235:CYS:H     | 1.66                     | 0.60              |
| 10:j:12:GLN:NE2  | 19:h:502:MGD:H8   | 2.17                     | 0.60              |
| 9:g:127:LEU:HD21 | 12:h:406:VAL:HG22 | 1.83                     | 0.59              |
| 4:C:143:ASP:OD1  | 4:C:144:VAL:N     | 2.36                     | 0.59              |
| 2:f:135:ILE:HG22 | 2:f:139:LYS:HE3   | 1.84                     | 0.59              |
| 7:I:13:GLU:OE2   | 12:H:86:LYS:NZ    | 2.34                     | 0.59              |
| 9:G:76:ASP:HA    | 9:G:84:ARG:HH22   | 1.67                     | 0.59              |
| 1:a:17:GLY:O     | 1:a:18:THR:HG22   | 2.03                     | 0.59              |
| 1:A:17:GLY:O     | 1:A:18:THR:HG22   | 2.03                     | 0.59              |
| 10:J:12:GLN:NE2  | 19:H:502:MGD:H8   | 2.17                     | 0.59              |
| 6:d:310:SER:HA   | 6:d:313:ASN:HD22  | 1.66                     | 0.59              |
| 12:h:293:MET:HA  | 12:h:403:MET:HE3  | 1.85                     | 0.59              |
| 7:I:145:ARG:NH1  | 9:G:75:GLU:OE2    | 2.36                     | 0.59              |
| 11:K:305:ALA:O   | 11:K:306:LYS:HG2  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:c:143:ASP:OD1   | 4:c:144:VAL:N     | 2.36                     | 0.59              |
| 4:c:61:SER:OG     | 4:c:84:ASP:OD2    | 2.20                     | 0.59              |
| 9:G:110:TYR:CE2   | 9:G:118:THR:HG21  | 2.38                     | 0.59              |
| 9:G:525:LYS:HB3   | 9:G:567:GLU:HA    | 1.85                     | 0.59              |
| 7:i:13:GLU:OE2    | 12:h:86:LYS:NZ    | 2.34                     | 0.59              |
| 9:G:338:ILE:HG22  | 9:G:339:LYS:H     | 1.66                     | 0.59              |
| 1:a:498:VAL:HG12  | 4:c:20:TYR:HB3    | 1.85                     | 0.59              |
| 9:g:76:ASP:HA     | 9:g:84:ARG:HH22   | 1.67                     | 0.59              |
| 2:F:135:ILE:HG22  | 2:F:139:LYS:HE3   | 1.84                     | 0.59              |
| 9:g:73:ARG:HG2    | 9:g:76:ASP:HB2    | 1.85                     | 0.59              |
| 9:g:338:ILE:HG22  | 9:g:339:LYS:H     | 1.66                     | 0.59              |
| 11:k:305:ALA:O    | 11:k:306:LYS:HG2  | 2.02                     | 0.59              |
| 12:H:256:THR:HB   | 12:H:290:ILE:HD12 | 1.85                     | 0.58              |
| 12:H:293:MET:HA   | 12:H:403:MET:HE3  | 1.85                     | 0.58              |
| 7:i:145:ARG:NH1   | 9:g:75:GLU:OE2    | 2.36                     | 0.58              |
| 9:g:525:LYS:HB3   | 9:g:567:GLU:HA    | 1.85                     | 0.58              |
| 11:m:194:PHE:HE1  | 11:m:201:VAL:HG23 | 1.68                     | 0.58              |
| 9:G:150:GLY:HA3   | 9:G:185:VAL:HG13  | 1.85                     | 0.58              |
| 9:G:186:VAL:HG13  | 9:G:237:HIS:ND1   | 2.16                     | 0.58              |
| 2:f:61:ASP:OD1    | 2:f:136:LYS:NZ    | 2.34                     | 0.58              |
| 9:g:73:ARG:NH2    | 9:g:318:GLU:OE1   | 2.37                     | 0.58              |
| 8:L:92:THR:HG23   | 11:K:280:LYS:HA   | 1.85                     | 0.58              |
| 9:G:73:ARG:NH2    | 9:G:318:GLU:OE1   | 2.37                     | 0.58              |
| 8:l:118:LEU:HD23  | 11:k:371:VAL:HG12 | 1.84                     | 0.58              |
| 9:g:110:TYR:CE2   | 9:g:118:THR:HG21  | 2.38                     | 0.58              |
| 12:h:94:GLY:HA2   | 12:h:299:ILE:HD13 | 1.85                     | 0.58              |
| 3:E:79:LEU:HD12   | 3:E:104:ASP:OD1   | 2.03                     | 0.58              |
| 3:e:79:LEU:HD12   | 3:e:104:ASP:OD1   | 2.03                     | 0.58              |
| 1:A:20:ILE:HG22   | 1:A:26:ILE:HD11   | 1.84                     | 0.58              |
| 8:L:118:LEU:HD23  | 11:K:371:VAL:HG12 | 1.84                     | 0.58              |
| 1:a:20:ILE:HG22   | 1:a:26:ILE:HD11   | 1.84                     | 0.58              |
| 6:D:73:LYS:HD3    | 6:D:78:ILE:HD11   | 1.85                     | 0.58              |
| 4:c:10:GLU:HG2    | 4:c:11:LEU:HD12   | 1.85                     | 0.58              |
| 1:A:168:SER:O     | 1:a:583:MET:HE2   | 2.04                     | 0.58              |
| 11:M:194:PHE:HE1  | 11:M:201:VAL:HG23 | 1.68                     | 0.58              |
| 9:G:523:TRP:CE2   | 9:G:565:ALA:HB2   | 2.39                     | 0.58              |
| 9:g:150:GLY:HA3   | 9:g:185:VAL:HG13  | 1.85                     | 0.58              |
| 9:G:73:ARG:HG2    | 9:G:76:ASP:HB2    | 1.85                     | 0.57              |
| 12:h:128:LEU:HD21 | 12:h:328:PRO:HG2  | 1.86                     | 0.57              |
| 12:h:256:THR:HB   | 12:h:290:ILE:HD12 | 1.85                     | 0.57              |
| 4:C:10:GLU:HG2    | 4:C:11:LEU:HD12   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:137:CYS:SG    | 6:D:401:LEU:HD21  | 2.45                     | 0.57              |
| 7:I:129:GLU:HG3   | 7:I:155:LYS:HD3   | 1.87                     | 0.57              |
| 1:A:498:VAL:HG12  | 4:C:20:TYR:HB3    | 1.85                     | 0.57              |
| 3:E:195:MET:HE2   | 3:E:198:PRO:HA    | 1.86                     | 0.57              |
| 9:G:462:TYR:OH    | 9:G:564:ARG:NH2   | 2.37                     | 0.57              |
| 6:D:140:ILE:HD13  | 6:D:407:TYR:CE2   | 2.38                     | 0.57              |
| 6:D:444:ALA:HB1   | 6:D:448:GLU:HB2   | 1.86                     | 0.57              |
| 1:a:327:GLU:O     | 1:a:329:GLN:NE2   | 2.38                     | 0.57              |
| 7:I:129:GLU:HA    | 7:I:155:LYS:HB2   | 1.86                     | 0.57              |
| 12:H:94:GLY:HA2   | 12:H:299:ILE:HD13 | 1.85                     | 0.57              |
| 3:e:195:MET:HE2   | 3:e:198:PRO:HA    | 1.86                     | 0.57              |
| 9:g:523:TRP:CE2   | 9:g:565:ALA:HB2   | 2.39                     | 0.57              |
| 1:a:16:CYS:HB2    | 13:a:703:SF4:S4   | 2.45                     | 0.57              |
| 6:d:140:ILE:HD13  | 6:d:407:TYR:CE2   | 2.38                     | 0.57              |
| 7:i:129:GLU:HA    | 7:i:155:LYS:HB2   | 1.86                     | 0.57              |
| 12:H:128:LEU:HD21 | 12:H:328:PRO:HG2  | 1.86                     | 0.57              |
| 9:G:277:ILE:HD12  | 9:G:309:CYS:HB3   | 1.87                     | 0.57              |
| 8:l:92:THR:HG23   | 11:k:280:LYS:HA   | 1.85                     | 0.57              |
| 9:g:462:TYR:OH    | 9:g:564:ARG:NH2   | 2.37                     | 0.57              |
| 10:j:9:MET:HE1    | 10:j:82:ILE:HD12  | 1.87                     | 0.57              |
| 1:A:16:CYS:HB2    | 13:A:703:SF4:S4   | 2.45                     | 0.56              |
| 6:d:266:ALA:HB3   | 6:d:270:HIS:HE2   | 1.70                     | 0.56              |
| 1:A:583:MET:HE2   | 1:a:168:SER:O     | 2.05                     | 0.56              |
| 8:L:140:PRO:HA    | 11:K:379:GLY:HA3  | 1.87                     | 0.56              |
| 9:G:274:ASN:HB3   | 9:G:277:ILE:HD11  | 1.87                     | 0.56              |
| 10:J:88:ALA:O     | 10:J:92:VAL:HG23  | 2.05                     | 0.56              |
| 6:d:137:CYS:SG    | 6:d:401:LEU:HD21  | 2.45                     | 0.56              |
| 9:g:274:ASN:HB3   | 9:g:277:ILE:HD11  | 1.87                     | 0.56              |
| 1:A:235:ASP:OD2   | 1:A:336:LYS:NZ    | 2.37                     | 0.56              |
| 12:H:71:TYR:O     | 12:H:75:ILE:HG12  | 2.06                     | 0.56              |
| 9:G:138:THR:HG21  | 9:G:143:GLN:HE22  | 1.70                     | 0.56              |
| 1:a:235:ASP:OD2   | 1:a:336:LYS:NZ    | 2.37                     | 0.56              |
| 7:i:129:GLU:HG3   | 7:i:155:LYS:HD3   | 1.86                     | 0.56              |
| 11:k:326:CYS:SG   | 11:k:327:GLY:N    | 2.79                     | 0.56              |
| 6:d:73:LYS:HD3    | 6:d:78:ILE:HD11   | 1.85                     | 0.56              |
| 8:l:140:PRO:HA    | 11:k:379:GLY:HA3  | 1.87                     | 0.56              |
| 9:g:138:THR:HG21  | 9:g:143:GLN:HE22  | 1.70                     | 0.56              |
| 12:h:71:TYR:O     | 12:h:75:ILE:HG12  | 2.06                     | 0.56              |
| 8:L:105:ILE:HG23  | 12:H:35:GLU:HG2   | 1.88                     | 0.56              |
| 8:l:105:ILE:HG23  | 12:h:35:GLU:HG2   | 1.88                     | 0.56              |
| 11:m:222:CYS:SG   | 11:m:224:SER:O    | 2.64                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:327:GLU:O    | 1:A:329:GLN:NE2   | 2.38                     | 0.56              |
| 6:d:107:PHE:CZ   | 6:d:129:PHE:HZ    | 2.24                     | 0.56              |
| 9:G:531:ASN:HB2  | 9:G:534:VAL:HG22  | 1.88                     | 0.56              |
| 6:D:266:ALA:HB3  | 6:D:270:HIS:HE2   | 1.71                     | 0.56              |
| 11:K:326:CYS:SG  | 11:K:327:GLY:N    | 2.79                     | 0.56              |
| 12:H:312:PHE:HB2 | 12:H:316:LEU:HD21 | 1.88                     | 0.56              |
| 1:a:282:GLY:HA3  | 11:k:6:PRO:HD3    | 1.88                     | 0.56              |
| 6:d:444:ALA:HB1  | 6:d:448:GLU:HB2   | 1.86                     | 0.56              |
| 11:K:298:TYR:CE1 | 11:K:317:ALA:HB3  | 2.41                     | 0.55              |
| 6:d:403:PRO:HB3  | 6:d:407:TYR:CE1   | 2.41                     | 0.55              |
| 12:h:312:PHE:HB2 | 12:h:316:LEU:HD21 | 1.87                     | 0.55              |
| 6:D:107:PHE:CZ   | 6:D:129:PHE:HZ    | 2.24                     | 0.55              |
| 9:g:277:ILE:HD12 | 9:g:309:CYS:HB3   | 1.87                     | 0.55              |
| 10:j:88:ALA:O    | 10:j:92:VAL:HG23  | 2.05                     | 0.55              |
| 11:k:298:TYR:CE1 | 11:k:317:ALA:HB3  | 2.41                     | 0.55              |
| 1:A:218:MET:HE3  | 1:A:298:PRO:HG3   | 1.88                     | 0.55              |
| 10:J:9:MET:HE1   | 10:J:82:ILE:HD12  | 1.87                     | 0.55              |
| 12:H:140:LEU:HG  | 12:H:291:MET:HE1  | 1.88                     | 0.55              |
| 1:A:189:LEU:HA   | 1:A:372:GLU:HG2   | 1.89                     | 0.55              |
| 9:G:65:LYS:HZ1   | 9:G:324:ALA:HB2   | 1.72                     | 0.55              |
| 9:G:242:GLY:HA2  | 9:G:282:TYR:HE1   | 1.72                     | 0.55              |
| 3:e:253:ILE:O    | 3:e:257:VAL:HG23  | 2.07                     | 0.55              |
| 11:M:222:CYS:SG  | 11:M:224:SER:O    | 2.64                     | 0.55              |
| 1:a:556:VAL:HG13 | 1:a:560:PRO:HA    | 1.88                     | 0.55              |
| 12:h:14:GLY:O    | 12:h:403:MET:HG3  | 2.06                     | 0.55              |
| 7:I:204:MET:O    | 7:I:250:LYS:NZ    | 2.40                     | 0.55              |
| 6:d:426:GLN:NE2  | 6:d:479:ILE:HD12  | 2.22                     | 0.55              |
| 9:g:242:GLY:HA2  | 9:g:282:TYR:HE1   | 1.72                     | 0.55              |
| 7:i:242:PHE:HB2  | 7:i:262:ILE:HG23  | 1.89                     | 0.55              |
| 11:k:342:ARG:HG3 | 11:k:366:PRO:HB3  | 1.89                     | 0.55              |
| 1:A:282:GLY:HA3  | 11:K:6:PRO:HD3    | 1.88                     | 0.55              |
| 1:A:556:VAL:HG13 | 1:A:560:PRO:HA    | 1.88                     | 0.55              |
| 3:E:253:ILE:O    | 3:E:257:VAL:HG23  | 2.07                     | 0.55              |
| 1:a:225:GLU:OE2  | 1:a:239:ARG:NE    | 2.38                     | 0.55              |
| 7:i:250:LYS:HB2  | 7:i:257:ILE:HD11  | 1.88                     | 0.55              |
| 6:D:426:GLN:NE2  | 6:D:479:ILE:HD12  | 2.22                     | 0.55              |
| 12:H:291:MET:HE3 | 12:H:404:ASP:HB3  | 1.89                     | 0.55              |
| 7:i:253:LYS:HG3  | 7:i:254:LYS:N     | 2.22                     | 0.55              |
| 6:D:403:PRO:HB3  | 6:D:407:TYR:CE1   | 2.41                     | 0.54              |
| 7:i:204:MET:O    | 7:i:250:LYS:NZ    | 2.40                     | 0.54              |
| 9:g:531:ASN:HB2  | 9:g:534:VAL:HG22  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:k:351:LYS:HG3 | 11:k:352:GLU:H   | 1.72                     | 0.54              |
| 7:i:28:GLY:N     | 7:i:59:GLY:O     | 2.40                     | 0.54              |
| 3:E:180:GLU:HG2  | 3:E:191:ARG:HH21 | 1.71                     | 0.54              |
| 1:a:189:LEU:HA   | 1:a:372:GLU:HG2  | 1.88                     | 0.54              |
| 1:a:218:MET:HE3  | 1:a:298:PRO:HG3  | 1.88                     | 0.54              |
| 12:h:16:SER:HB2  | 12:h:402:ARG:HG3 | 1.89                     | 0.54              |
| 12:h:140:LEU:HG  | 12:h:291:MET:HE1 | 1.88                     | 0.54              |
| 6:D:398:ILE:HG23 | 6:D:401:LEU:HB2  | 1.88                     | 0.54              |
| 12:H:125:PRO:HB3 | 12:H:268:ARG:HB3 | 1.90                     | 0.54              |
| 3:e:180:GLU:HG2  | 3:e:191:ARG:HH21 | 1.71                     | 0.54              |
| 9:G:387:ILE:CG1  | 9:G:447:MET:HE2  | 2.36                     | 0.54              |
| 10:j:8:ASN:OD1   | 10:j:9:MET:N     | 2.41                     | 0.54              |
| 10:J:8:ASN:OD1   | 10:J:9:MET:N     | 2.40                     | 0.54              |
| 4:c:175:ILE:HG23 | 4:c:180:LEU:HB3  | 1.89                     | 0.54              |
| 5:B:84:LYS:NZ    | 5:B:88:GLU:OE1   | 2.41                     | 0.54              |
| 6:D:129:PHE:HD2  | 6:D:131:THR:CG2  | 2.21                     | 0.54              |
| 6:D:141:CYS:SG   | 6:D:142:HIS:N    | 2.81                     | 0.54              |
| 9:g:275:THR:O    | 9:g:276:HIS:C    | 2.51                     | 0.54              |
| 12:h:291:MET:HE3 | 12:h:404:ASP:HB3 | 1.89                     | 0.54              |
| 7:I:250:LYS:HB2  | 7:I:257:ILE:HD11 | 1.88                     | 0.54              |
| 12:H:14:GLY:O    | 12:H:403:MET:HG3 | 2.06                     | 0.54              |
| 5:b:84:LYS:NZ    | 5:b:88:GLU:OE1   | 2.41                     | 0.54              |
| 7:I:2:GLU:N      | 7:I:57:LYS:O     | 2.41                     | 0.54              |
| 7:I:242:PHE:HB2  | 7:I:262:ILE:HG23 | 1.89                     | 0.54              |
| 9:G:159:ILE:HG22 | 9:G:212:ILE:HD11 | 1.90                     | 0.54              |
| 12:H:76:ASP:OD1  | 12:H:433:ARG:NH2 | 2.41                     | 0.54              |
| 11:k:147:PHE:HA  | 11:k:154:GLY:H   | 1.73                     | 0.54              |
| 9:G:149:PHE:CE2  | 9:G:174:LEU:HD23 | 2.43                     | 0.54              |
| 11:k:148:GLU:OE1 | 11:k:148:GLU:N   | 2.40                     | 0.54              |
| 4:C:175:ILE:HG23 | 4:C:180:LEU:HB3  | 1.89                     | 0.53              |
| 7:I:253:LYS:HG3  | 7:I:254:LYS:N    | 2.22                     | 0.53              |
| 11:M:180:CYS:SG  | 11:M:181:GLY:N   | 2.81                     | 0.53              |
| 12:H:16:SER:HB2  | 12:H:402:ARG:HG3 | 1.89                     | 0.53              |
| 6:d:141:CYS:SG   | 6:d:142:HIS:N    | 2.81                     | 0.53              |
| 6:d:398:ILE:HG23 | 6:d:401:LEU:HB2  | 1.88                     | 0.53              |
| 12:h:76:ASP:OD1  | 12:h:433:ARG:NH2 | 2.41                     | 0.53              |
| 6:D:202:VAL:HG12 | 6:D:202:VAL:O    | 2.09                     | 0.53              |
| 9:G:275:THR:O    | 9:G:276:HIS:C    | 2.51                     | 0.53              |
| 1:A:93:ASN:OD1   | 1:A:94:PRO:HD2   | 2.08                     | 0.53              |
| 11:K:342:ARG:HG3 | 11:K:366:PRO:HB3 | 1.89                     | 0.53              |
| 11:K:351:LYS:HG3 | 11:K:352:GLU:H   | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:d:335:ASN:OD1   | 6:d:336:ASN:N     | 2.42                     | 0.53              |
| 1:A:225:GLU:OE2   | 1:A:239:ARG:NE    | 2.38                     | 0.53              |
| 6:D:335:ASN:OD1   | 6:D:336:ASN:N     | 2.42                     | 0.53              |
| 12:h:125:PRO:HB3  | 12:h:268:ARG:HB3  | 1.90                     | 0.53              |
| 12:h:143:VAL:HG11 | 12:h:255:THR:HG21 | 1.90                     | 0.53              |
| 3:E:110:GLU:OE2   | 3:E:113:LYS:NZ    | 2.33                     | 0.53              |
| 6:D:365:MET:HE1   | 6:D:507:VAL:HG13  | 1.90                     | 0.53              |
| 10:J:41:GLU:HG3   | 10:J:70:VAL:HG21  | 1.91                     | 0.53              |
| 12:H:320:LYS:HG3  | 12:H:323:HIS:NE2  | 2.24                     | 0.53              |
| 6:d:358:VAL:HG23  | 6:d:361:ASN:OD1   | 2.09                     | 0.53              |
| 9:g:149:PHE:CE2   | 9:g:174:LEU:HD23  | 2.43                     | 0.53              |
| 11:m:180:CYS:SG   | 11:m:181:GLY:N    | 2.81                     | 0.53              |
| 11:K:19:MET:SD    | 11:K:73:VAL:HB    | 2.49                     | 0.53              |
| 12:H:12:TYR:HB2   | 12:H:44:ILE:CD1   | 2.39                     | 0.53              |
| 6:d:202:VAL:HG12  | 6:d:202:VAL:O     | 2.09                     | 0.53              |
| 11:k:19:MET:SD    | 11:k:73:VAL:HB    | 2.49                     | 0.53              |
| 4:C:152:LEU:HD21  | 5:B:280:ALA:HB2   | 1.91                     | 0.53              |
| 5:B:214:ASP:OD2   | 4:c:2:ALA:N       | 2.41                     | 0.53              |
| 6:D:358:VAL:HG23  | 6:D:361:ASN:OD1   | 2.09                     | 0.53              |
| 8:L:130:PRO:HA    | 12:H:199:VAL:HG23 | 1.90                     | 0.53              |
| 1:a:93:ASN:OD1    | 1:a:94:PRO:HD2    | 2.08                     | 0.53              |
| 9:g:308:THR:OG1   | 9:g:384:ARG:O     | 2.21                     | 0.53              |
| 9:g:387:ILE:CG1   | 9:g:447:MET:HE2   | 2.36                     | 0.53              |
| 1:A:297:MET:HB3   | 1:A:298:PRO:HD3   | 1.91                     | 0.53              |
| 7:i:2:GLU:N       | 7:i:57:LYS:O      | 2.41                     | 0.53              |
| 8:L:103:LYS:HB2   | 8:L:112:LEU:HD11  | 1.90                     | 0.53              |
| 10:J:103:GLN:HA   | 12:H:268:ARG:HH22 | 1.74                     | 0.53              |
| 6:d:516:TYR:CD1   | 6:d:519:LEU:HD12  | 2.44                     | 0.53              |
| 10:j:103:GLN:HA   | 12:h:268:ARG:HH22 | 1.74                     | 0.53              |
| 9:G:147:PRO:HD3   | 9:G:180:GLY:HA3   | 1.91                     | 0.53              |
| 11:K:147:PHE:HA   | 11:K:154:GLY:H    | 1.73                     | 0.53              |
| 12:h:320:LYS:HG3  | 12:h:323:HIS:NE2  | 2.24                     | 0.53              |
| 12:h:12:TYR:HB2   | 12:h:44:ILE:CD1   | 2.39                     | 0.52              |
| 4:C:149:ARG:NH1   | 5:B:20:GLU:OE2    | 2.42                     | 0.52              |
| 7:I:28:GLY:N      | 7:I:59:GLY:O      | 2.40                     | 0.52              |
| 8:l:103:LYS:HB2   | 8:l:112:LEU:HD11  | 1.90                     | 0.52              |
| 4:C:2:ALA:N       | 5:b:214:ASP:OD2   | 2.43                     | 0.52              |
| 5:B:233:GLU:CD    | 5:B:239:GLN:HB2   | 2.35                     | 0.52              |
| 6:D:342:ASP:HB3   | 6:D:511:MET:HE1   | 1.90                     | 0.52              |
| 12:H:373:ASP:HB2  | 12:H:386:HIS:HE1  | 1.75                     | 0.52              |
| 11:k:236:GLN:C    | 11:k:237:LYS:HD3  | 2.35                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:20:ILE:HD11   | 1:A:103:ARG:HB2   | 1.90                     | 0.52              |
| 9:G:96:MET:HE3    | 9:G:96:MET:HA     | 1.91                     | 0.52              |
| 12:H:143:VAL:HG11 | 12:H:255:THR:HG21 | 1.90                     | 0.52              |
| 3:e:324:LEU:HG    | 6:d:208:MET:SD    | 2.49                     | 0.52              |
| 4:c:149:ARG:NH1   | 5:b:20:GLU:OE2    | 2.42                     | 0.52              |
| 6:d:407:TYR:HB2   | 6:d:413:VAL:HG21  | 1.90                     | 0.52              |
| 9:g:96:MET:HE3    | 9:g:96:MET:HA     | 1.91                     | 0.52              |
| 9:g:159:ILE:HG22  | 9:g:212:ILE:HD11  | 1.90                     | 0.52              |
| 1:a:281:MET:HE3   | 1:a:369:LEU:HD13  | 1.92                     | 0.52              |
| 1:a:521:ARG:HB3   | 1:a:534:MET:HE2   | 1.92                     | 0.52              |
| 3:e:112:ALA:HB3   | 3:e:381:MET:HE1   | 1.92                     | 0.52              |
| 6:d:70:LEU:HB3    | 6:d:77:PHE:HB3    | 1.90                     | 0.52              |
| 10:j:40:ASN:HD22  | 10:j:77:PRO:HA    | 1.75                     | 0.52              |
| 3:E:177:ASP:O     | 3:E:181:GLU:HG2   | 2.09                     | 0.52              |
| 12:H:211:ASP:OD1  | 19:H:502:MGD:N1   | 2.43                     | 0.52              |
| 3:e:177:ASP:O     | 3:e:181:GLU:HG2   | 2.09                     | 0.52              |
| 6:d:342:ASP:HB3   | 6:d:511:MET:HE1   | 1.90                     | 0.52              |
| 6:D:70:LEU:HB3    | 6:D:77:PHE:HB3    | 1.90                     | 0.52              |
| 6:D:516:TYR:CD1   | 6:D:519:LEU:HD12  | 2.44                     | 0.52              |
| 9:G:110:TYR:CB    | 9:G:141:LEU:HD21  | 2.40                     | 0.52              |
| 8:l:103:LYS:HE3   | 8:l:105:ILE:HD11  | 1.92                     | 0.52              |
| 12:h:211:ASP:OD1  | 19:h:502:MGD:N1   | 2.43                     | 0.52              |
| 6:D:407:TYR:HB2   | 6:D:413:VAL:HG21  | 1.90                     | 0.52              |
| 8:l:130:PRO:HA    | 12:h:199:VAL:HG23 | 1.90                     | 0.52              |
| 10:j:41:GLU:HG3   | 10:j:70:VAL:HG21  | 1.91                     | 0.52              |
| 9:g:67:ASN:ND2    | 9:g:70:ARG:HH11   | 2.08                     | 0.52              |
| 9:g:186:VAL:HA    | 9:g:237:HIS:HB2   | 1.91                     | 0.52              |
| 12:h:373:ASP:HB2  | 12:h:386:HIS:HE1  | 1.75                     | 0.52              |
| 3:E:324:LEU:HG    | 6:D:208:MET:SD    | 2.49                     | 0.52              |
| 11:K:276:PHE:CD2  | 11:K:318:VAL:HB   | 2.45                     | 0.52              |
| 4:c:152:LEU:HD21  | 5:b:280:ALA:HB2   | 1.91                     | 0.52              |
| 6:d:365:MET:HE1   | 6:d:507:VAL:HG13  | 1.91                     | 0.52              |
| 10:j:44:MET:HE1   | 10:j:51:LYS:HG2   | 1.92                     | 0.52              |
| 12:h:260:MET:SD   | 12:h:260:MET:N    | 2.83                     | 0.52              |
| 1:A:110:HIS:CD2   | 2:F:34:PRO:HB3    | 2.45                     | 0.51              |
| 6:D:323:ARG:HA    | 6:D:542:ARG:NH2   | 2.24                     | 0.51              |
| 9:G:186:VAL:HA    | 9:G:237:HIS:HB2   | 1.91                     | 0.51              |
| 8:l:90:LEU:O      | 9:g:544:LYS:NZ    | 2.43                     | 0.51              |
| 9:g:110:TYR:CB    | 9:g:141:LEU:HD21  | 2.40                     | 0.51              |
| 9:g:147:PRO:HD3   | 9:g:180:GLY:HA3   | 1.91                     | 0.51              |
| 1:A:281:MET:HE3   | 1:A:369:LEU:HD13  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:E:33:HIS:O     | 3:E:37:THR:HG22   | 2.10                     | 0.51              |
| 3:E:53:TYR:N     | 3:E:53:TYR:HD2    | 2.08                     | 0.51              |
| 9:G:110:TYR:CD2  | 9:G:118:THR:HG21  | 2.45                     | 0.51              |
| 1:a:297:MET:HB3  | 1:a:298:PRO:HD3   | 1.91                     | 0.51              |
| 4:c:26:ASN:HB3   | 4:c:29:PHE:HB3    | 1.92                     | 0.51              |
| 6:d:36:VAL:HG23  | 6:d:57:TRP:HB3    | 1.92                     | 0.51              |
| 6:d:323:ARG:HA   | 6:d:542:ARG:NH2   | 2.24                     | 0.51              |
| 7:i:39:ALA:O     | 7:i:46:TRP:N      | 2.42                     | 0.51              |
| 4:C:45:TYR:HE2   | 1:a:445:MET:SD    | 2.33                     | 0.51              |
| 10:J:40:ASN:HD22 | 10:J:77:PRO:HA    | 1.75                     | 0.51              |
| 3:e:53:TYR:HD2   | 3:e:53:TYR:N      | 2.08                     | 0.51              |
| 5:b:155:TYR:CZ   | 5:b:177:PHE:HB3   | 2.45                     | 0.51              |
| 5:b:233:GLU:CD   | 5:b:239:GLN:HB2   | 2.35                     | 0.51              |
| 9:g:160:LYS:HD3  | 9:g:210:PHE:O     | 2.10                     | 0.51              |
| 4:C:26:ASN:HB3   | 4:C:29:PHE:HB3    | 1.92                     | 0.51              |
| 6:D:36:VAL:HG23  | 6:D:57:TRP:HB3    | 1.92                     | 0.51              |
| 8:L:90:LEU:O     | 9:G:544:LYS:NZ    | 2.43                     | 0.51              |
| 12:H:99:GLU:HG3  | 12:H:424:GLU:HG3  | 1.93                     | 0.51              |
| 1:a:110:HIS:CD2  | 2:f:34:PRO:HB3    | 2.46                     | 0.51              |
| 3:e:53:TYR:N     | 3:e:53:TYR:CD2    | 2.77                     | 0.51              |
| 3:E:53:TYR:N     | 3:E:53:TYR:CD2    | 2.77                     | 0.51              |
| 6:D:323:ARG:HA   | 6:D:542:ARG:HH22  | 1.76                     | 0.51              |
| 9:g:110:TYR:CD2  | 9:g:118:THR:HG21  | 2.46                     | 0.51              |
| 1:A:116:ASP:OD1  | 1:A:116:ASP:N     | 2.44                     | 0.51              |
| 3:E:141:MET:HE2  | 3:E:184:TYR:HB3   | 1.92                     | 0.51              |
| 5:B:77:LEU:HD13  | 5:B:83:TYR:HA     | 1.92                     | 0.51              |
| 11:K:148:GLU:OE2 | 11:K:157:LYS:N    | 2.44                     | 0.51              |
| 7:i:230:LYS:HB2  | 7:i:239:PHE:CD2   | 2.46                     | 0.51              |
| 11:k:276:PHE:CD2 | 11:k:318:VAL:HB   | 2.45                     | 0.51              |
| 12:h:179:LYS:HD2 | 12:h:183:LYS:HG3  | 1.92                     | 0.51              |
| 5:B:155:TYR:CZ   | 5:B:177:PHE:HB3   | 2.45                     | 0.51              |
| 7:I:227:THR:HA   | 7:I:240:ASP:HA    | 1.93                     | 0.51              |
| 10:J:90:GLN:HG3  | 10:J:125:LEU:HD22 | 1.92                     | 0.51              |
| 11:K:236:GLN:C   | 11:K:237:LYS:HD3  | 2.35                     | 0.51              |
| 5:b:216:THR:OG1  | 5:b:241:GLN:NE2   | 2.44                     | 0.51              |
| 9:g:110:TYR:HD2  | 9:g:141:LEU:HD13  | 1.76                     | 0.51              |
| 1:A:499:ASP:HB2  | 4:C:19:ARG:HD3    | 1.93                     | 0.51              |
| 3:E:112:ALA:HB3  | 3:E:381:MET:HE1   | 1.92                     | 0.51              |
| 6:D:234:TRP:HE1  | 6:D:274:LEU:HD11  | 1.76                     | 0.51              |
| 8:L:103:LYS:HE3  | 8:L:105:ILE:HD11  | 1.92                     | 0.51              |
| 12:H:179:LYS:HD2 | 12:H:183:LYS:HG3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:e:33:HIS:O     | 3:e:37:THR:HG22   | 2.10                     | 0.51              |
| 7:i:179:ILE:HG22 | 7:i:197:GLU:OE1   | 2.11                     | 0.51              |
| 12:h:111:ALA:HB2 | 12:h:434:MET:HE1  | 1.92                     | 0.51              |
| 5:B:157:CYS:HB2  | 16:B:302:9S8:S3   | 2.51                     | 0.51              |
| 9:G:382:LEU:HD12 | 9:G:447:MET:SD    | 2.51                     | 0.51              |
| 6:d:495:PRO:HD2  | 6:d:499:ASP:OD2   | 2.11                     | 0.51              |
| 11:k:148:GLU:OE2 | 11:k:157:LYS:N    | 2.44                     | 0.51              |
| 1:A:521:ARG:HB3  | 1:A:534:MET:HE2   | 1.92                     | 0.51              |
| 2:F:85:ARG:O     | 2:F:89:ILE:HG12   | 2.11                     | 0.51              |
| 6:D:250:VAL:HG12 | 6:D:554:LEU:HD22  | 1.93                     | 0.51              |
| 9:G:67:ASN:ND2   | 9:G:70:ARG:HH11   | 2.08                     | 0.51              |
| 9:G:143:GLN:O    | 9:G:521:THR:HA    | 2.11                     | 0.51              |
| 10:J:44:MET:HE1  | 10:J:51:LYS:HG2   | 1.92                     | 0.51              |
| 3:e:141:MET:HE2  | 3:e:184:TYR:HB3   | 1.92                     | 0.51              |
| 6:d:323:ARG:HA   | 6:d:542:ARG:HH22  | 1.76                     | 0.51              |
| 1:A:101:ASN:O    | 1:A:125:GLN:NE2   | 2.43                     | 0.50              |
| 7:I:230:LYS:HB2  | 7:I:239:PHE:CD2   | 2.46                     | 0.50              |
| 9:G:522:LEU:HD21 | 9:G:564:ARG:HH21  | 1.76                     | 0.50              |
| 6:d:129:PHE:HD2  | 6:d:131:THR:CG2   | 2.21                     | 0.50              |
| 10:j:90:GLN:HG3  | 10:j:125:LEU:HD22 | 1.92                     | 0.50              |
| 6:d:256:LEU:O    | 6:d:260:VAL:HG22  | 2.11                     | 0.50              |
| 9:g:143:GLN:O    | 9:g:521:THR:HA    | 2.11                     | 0.50              |
| 9:g:382:LEU:HD12 | 9:g:447:MET:SD    | 2.51                     | 0.50              |
| 12:h:99:GLU:HG3  | 12:h:424:GLU:HG3  | 1.93                     | 0.50              |
| 5:B:289:THR:O    | 5:B:293:GLN:HG2   | 2.12                     | 0.50              |
| 6:D:43:PRO:HG3   | 6:D:523:GLU:HA    | 1.93                     | 0.50              |
| 1:A:444:TYR:CD1  | 1:A:447:ILE:HG12  | 2.47                     | 0.50              |
| 1:A:445:MET:SD   | 4:c:45:TYR:HE2    | 2.34                     | 0.50              |
| 9:G:160:LYS:HD3  | 9:G:210:PHE:O     | 2.10                     | 0.50              |
| 6:d:250:VAL:HG12 | 6:d:554:LEU:HD22  | 1.93                     | 0.50              |
| 6:D:250:VAL:CG1  | 6:D:554:LEU:HD22  | 2.42                     | 0.50              |
| 10:J:37:ILE:HB   | 10:J:68:ALA:HA    | 1.94                     | 0.50              |
| 12:H:260:MET:SD  | 12:H:260:MET:N    | 2.83                     | 0.50              |
| 3:e:110:GLU:OE2  | 3:e:113:LYS:NZ    | 2.33                     | 0.50              |
| 5:b:157:CYS:HB2  | 16:b:302:9S8:S3   | 2.51                     | 0.50              |
| 9:g:11:ILE:HG13  | 9:g:23:ALA:HB3    | 1.94                     | 0.50              |
| 10:j:37:ILE:HB   | 10:j:68:ALA:HA    | 1.94                     | 0.50              |
| 11:k:161:VAL:HA  | 11:k:237:LYS:CG   | 2.41                     | 0.50              |
| 2:f:85:ARG:O     | 2:f:89:ILE:HG12   | 2.11                     | 0.50              |
| 6:d:234:TRP:HE1  | 6:d:274:LEU:HD11  | 1.76                     | 0.50              |
| 6:d:250:VAL:CG1  | 6:d:554:LEU:HD22  | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:i:227:THR:HA   | 7:i:240:ASP:HA   | 1.93                     | 0.50              |
| 9:g:241:LEU:HD11 | 9:g:279:PHE:HB3  | 1.94                     | 0.50              |
| 2:F:84:LYS:HD3   | 3:E:389:VAL:HG22 | 1.93                     | 0.50              |
| 6:D:323:ARG:O    | 6:D:326:VAL:HG12 | 2.12                     | 0.50              |
| 9:G:551:GLU:HG3  | 12:H:411:ARG:NH2 | 2.27                     | 0.50              |
| 1:a:101:ASN:O    | 1:a:125:GLN:NE2  | 2.43                     | 0.50              |
| 11:k:88:CYS:SG   | 11:k:90:PHE:O    | 2.69                     | 0.50              |
| 12:h:142:GLU:OE2 | 12:h:146:ARG:NE  | 2.38                     | 0.50              |
| 5:B:216:THR:OG1  | 5:B:241:GLN:NE2  | 2.44                     | 0.50              |
| 6:D:495:PRO:HD2  | 6:D:499:ASP:OD2  | 2.11                     | 0.50              |
| 3:e:324:LEU:O    | 3:e:326:THR:N    | 2.45                     | 0.50              |
| 7:I:184:HIS:H    | 7:I:203:GLN:HB2  | 1.77                     | 0.50              |
| 1:a:332:PHE:O    | 1:a:333:ILE:HD13 | 2.12                     | 0.50              |
| 5:b:77:LEU:HD13  | 5:b:83:TYR:HA    | 1.92                     | 0.50              |
| 9:g:237:HIS:CD2  | 9:g:276:HIS:HE1  | 2.30                     | 0.50              |
| 9:g:362:ILE:HG22 | 9:g:364:VAL:H    | 1.76                     | 0.50              |
| 6:D:67:THR:HG23  | 6:D:471:GLY:HA3  | 1.94                     | 0.49              |
| 6:D:174:TRP:CD2  | 6:D:311:MET:HE1  | 2.47                     | 0.49              |
| 6:D:256:LEU:O    | 6:D:260:VAL:HG22 | 2.12                     | 0.49              |
| 9:G:110:TYR:HD2  | 9:G:141:LEU:HD13 | 1.76                     | 0.49              |
| 12:H:111:ALA:HB2 | 12:H:434:MET:HE1 | 1.92                     | 0.49              |
| 6:d:129:PHE:CD2  | 6:d:131:THR:HG23 | 2.42                     | 0.49              |
| 3:E:78:LEU:H     | 3:E:78:LEU:HD23  | 1.77                     | 0.49              |
| 6:D:113:THR:HG22 | 6:D:117:ASP:HB2  | 1.95                     | 0.49              |
| 7:I:179:ILE:HG22 | 7:I:197:GLU:OE1  | 2.11                     | 0.49              |
| 9:G:362:ILE:HG22 | 9:G:364:VAL:H    | 1.76                     | 0.49              |
| 1:a:444:TYR:CD1  | 1:a:447:ILE:HG12 | 2.47                     | 0.49              |
| 3:e:78:LEU:HD23  | 3:e:78:LEU:H     | 1.77                     | 0.49              |
| 9:g:205:ASP:OD1  | 9:g:205:ASP:N    | 2.44                     | 0.49              |
| 9:g:522:LEU:HD21 | 9:g:564:ARG:HH21 | 1.76                     | 0.49              |
| 12:h:314:TYR:O   | 12:h:326:MET:HG3 | 2.12                     | 0.49              |
| 1:A:666:PHE:HZ   | 2:F:60:ALA:HB2   | 1.78                     | 0.49              |
| 3:E:324:LEU:O    | 3:E:326:THR:N    | 2.45                     | 0.49              |
| 6:D:516:TYR:HD1  | 6:D:519:LEU:HD12 | 1.78                     | 0.49              |
| 12:H:314:TYR:O   | 12:H:326:MET:HG3 | 2.12                     | 0.49              |
| 1:a:499:ASP:HB2  | 4:c:19:ARG:HD3   | 1.93                     | 0.49              |
| 6:d:323:ARG:O    | 6:d:326:VAL:HG12 | 2.12                     | 0.49              |
| 7:i:228:VAL:O    | 7:i:239:PHE:N    | 2.46                     | 0.49              |
| 1:A:158:ALA:HB2  | 1:A:566:THR:HG23 | 1.95                     | 0.49              |
| 1:A:332:PHE:O    | 1:A:333:ILE:HD13 | 2.12                     | 0.49              |
| 7:I:216:LEU:HG   | 7:I:217:TYR:CD2  | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:f:49:MET:HE1    | 3:e:386:HIS:NE2   | 2.27                     | 0.49              |
| 5:b:289:THR:O     | 5:b:293:GLN:HG2   | 2.11                     | 0.49              |
| 12:h:358:ILE:N    | 12:h:359:PRO:HD2  | 2.27                     | 0.49              |
| 4:C:126:LEU:O     | 4:C:130:GLN:HG2   | 2.13                     | 0.49              |
| 9:G:241:LEU:HD11  | 9:G:279:PHE:HB3   | 1.94                     | 0.49              |
| 11:K:88:CYS:SG    | 11:K:90:PHE:O     | 2.69                     | 0.49              |
| 12:H:358:ILE:N    | 12:H:359:PRO:HD2  | 2.27                     | 0.49              |
| 6:d:67:THR:HG23   | 6:d:471:GLY:HA3   | 1.94                     | 0.49              |
| 7:i:184:HIS:H     | 7:i:203:GLN:HB2   | 1.77                     | 0.49              |
| 1:A:34:LYS:HG3    | 1:A:42:ALA:HB3    | 1.94                     | 0.49              |
| 11:K:41:GLY:C     | 11:K:43:CYS:N     | 2.71                     | 0.49              |
| 1:a:158:ALA:HB2   | 1:a:566:THR:HG23  | 1.95                     | 0.49              |
| 7:i:216:LEU:HG    | 7:i:217:TYR:CD2   | 2.47                     | 0.49              |
| 4:C:185:ASP:OD1   | 4:C:186:ARG:N     | 2.46                     | 0.49              |
| 6:D:516:TYR:O     | 6:D:520:GLU:HG2   | 2.13                     | 0.49              |
| 9:G:322:MET:HG2   | 9:G:353:VAL:HG13  | 1.95                     | 0.49              |
| 6:d:174:TRP:CD2   | 6:d:311:MET:HE1   | 2.47                     | 0.49              |
| 6:d:516:TYR:HD1   | 6:d:519:LEU:HD12  | 1.78                     | 0.49              |
| 11:k:276:PHE:CE1  | 11:k:339:ILE:HG12 | 2.47                     | 0.49              |
| 7:I:139:ALA:HB2   | 7:I:146:GLY:HA3   | 1.94                     | 0.49              |
| 9:G:62:SER:OG     | 9:G:63:GLY:N      | 2.46                     | 0.49              |
| 9:G:237:HIS:CD2   | 9:G:276:HIS:HE1   | 2.30                     | 0.49              |
| 11:K:148:GLU:OE1  | 11:K:148:GLU:N    | 2.40                     | 0.49              |
| 11:K:276:PHE:CE1  | 11:K:339:ILE:HG12 | 2.47                     | 0.49              |
| 9:g:551:GLU:HG3   | 12:h:411:ARG:NH2  | 2.27                     | 0.49              |
| 11:k:18:ILE:HG12  | 11:k:31:ILE:HG12  | 1.94                     | 0.49              |
| 2:F:49:MET:HE1    | 3:E:386:HIS:NE2   | 2.27                     | 0.49              |
| 12:H:304:VAL:HG21 | 12:H:401:TYR:CE1  | 2.48                     | 0.49              |
| 2:f:84:LYS:HD3    | 3:e:389:VAL:HG22  | 1.93                     | 0.49              |
| 6:d:43:PRO:HG3    | 6:d:523:GLU:HA    | 1.93                     | 0.49              |
| 6:d:113:THR:HG22  | 6:d:117:ASP:HB2   | 1.94                     | 0.49              |
| 6:d:436:TYR:HD1   | 6:d:436:TYR:N     | 2.11                     | 0.49              |
| 1:a:473:VAL:HA    | 1:a:489:THR:HB    | 1.95                     | 0.49              |
| 9:g:219:LYS:O     | 9:g:223:GLU:HG3   | 2.13                     | 0.49              |
| 12:h:18:ASP:OD1   | 12:h:18:ASP:N     | 2.44                     | 0.49              |
| 7:I:228:VAL:O     | 7:I:239:PHE:N     | 2.46                     | 0.48              |
| 9:G:205:ASP:OD1   | 9:G:205:ASP:N     | 2.44                     | 0.48              |
| 12:H:18:ASP:OD1   | 12:H:18:ASP:N     | 2.44                     | 0.48              |
| 9:g:523:TRP:NE1   | 9:g:563:PRO:HB2   | 2.28                     | 0.48              |
| 1:A:93:ASN:HD22   | 1:A:138:ASP:HA    | 1.78                     | 0.48              |
| 1:A:388:PRO:HB3   | 11:K:5:PHE:CZ     | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:I:39:ALA:O     | 7:I:46:TRP:N     | 2.42                     | 0.48              |
| 9:G:11:ILE:HG13  | 9:G:23:ALA:HB3   | 1.94                     | 0.48              |
| 9:G:219:LYS:O    | 9:G:223:GLU:HG3  | 2.13                     | 0.48              |
| 11:K:18:ILE:HG12 | 11:K:31:ILE:HG12 | 1.95                     | 0.48              |
| 7:i:182:LEU:HD12 | 7:i:209:ALA:HB2  | 1.95                     | 0.48              |
| 6:D:107:PHE:HD1  | 6:D:121:PHE:CZ   | 2.31                     | 0.48              |
| 9:G:58:HIS:HE1   | 9:G:184:KCX:HE2  | 1.78                     | 0.48              |
| 10:J:93:PRO:HG2  | 10:J:103:GLN:HB3 | 1.94                     | 0.48              |
| 12:H:114:MET:HE1 | 12:H:317:ASP:OD1 | 2.14                     | 0.48              |
| 9:g:322:MET:HG2  | 9:g:353:VAL:HG13 | 1.95                     | 0.48              |
| 12:h:421:MET:HE1 | 12:h:429:LYS:HE2 | 1.95                     | 0.48              |
| 11:K:161:VAL:HA  | 11:K:237:LYS:CG  | 2.41                     | 0.48              |
| 1:a:666:PHE:HZ   | 2:f:60:ALA:HB2   | 1.78                     | 0.48              |
| 3:e:159:ASP:HB3  | 3:e:164:ILE:HD13 | 1.96                     | 0.48              |
| 4:c:126:LEU:O    | 4:c:130:GLN:HG2  | 2.13                     | 0.48              |
| 6:d:516:TYR:O    | 6:d:520:GLU:HG2  | 2.13                     | 0.48              |
| 9:g:58:HIS:HE1   | 9:g:184:KCX:HE2  | 1.78                     | 0.48              |
| 1:A:605:MET:HE3  | 1:A:642:PHE:HZ   | 1.78                     | 0.48              |
| 5:B:133:CYS:SG   | 5:B:137:LYS:HB3  | 2.54                     | 0.48              |
| 11:K:52:ILE:HG12 | 11:K:73:VAL:HG22 | 1.96                     | 0.48              |
| 1:a:93:ASN:HD22  | 1:a:138:ASP:HA   | 1.78                     | 0.48              |
| 6:d:326:VAL:HG22 | 6:d:327:GLY:H    | 1.79                     | 0.48              |
| 7:i:139:ALA:HB2  | 7:i:146:GLY:HA3  | 1.94                     | 0.48              |
| 1:A:16:CYS:HA    | 13:A:703:SF4:S1  | 2.54                     | 0.48              |
| 6:D:366:GLU:HG2  | 6:D:374:LEU:HD23 | 1.96                     | 0.48              |
| 1:a:34:LYS:HG3   | 1:a:42:ALA:HB3   | 1.95                     | 0.48              |
| 3:e:152:THR:CG2  | 3:e:168:GLU:HG3  | 2.43                     | 0.48              |
| 12:h:114:MET:HE1 | 12:h:317:ASP:OD1 | 2.14                     | 0.48              |
| 3:E:159:ASP:HB3  | 3:E:164:ILE:HD13 | 1.96                     | 0.48              |
| 4:C:49:THR:HG23  | 1:a:474:ALA:HA   | 1.96                     | 0.48              |
| 5:B:189:ILE:HD11 | 5:B:228:ALA:HB2  | 1.95                     | 0.48              |
| 3:e:15:ALA:O     | 3:e:19:LYS:HG2   | 2.14                     | 0.48              |
| 3:E:40:VAL:HG11  | 3:E:97:ALA:HB2   | 1.96                     | 0.48              |
| 7:I:203:GLN:N    | 7:I:245:ASP:OD1  | 2.47                     | 0.48              |
| 1:a:16:CYS:HA    | 13:a:703:SF4:S1  | 2.54                     | 0.48              |
| 1:a:605:MET:HE3  | 1:a:642:PHE:HZ   | 1.78                     | 0.48              |
| 9:g:62:SER:OG    | 9:g:63:GLY:N     | 2.46                     | 0.48              |
| 9:G:49:THR:HG21  | 9:G:441:LEU:HD21 | 1.95                     | 0.48              |
| 9:G:410:GLU:O    | 9:G:414:LYS:HG3  | 2.14                     | 0.48              |
| 10:j:93:PRO:HG2  | 10:j:103:GLN:HB3 | 1.94                     | 0.48              |
| 12:h:418:GLU:HG2 | 12:h:418:GLU:O   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:152:THR:CG2   | 3:E:168:GLU:HG3   | 2.43                     | 0.48              |
| 6:D:344:GLY:HA3   | 6:D:350:TYR:O     | 2.14                     | 0.48              |
| 6:D:436:TYR:CD1   | 6:D:436:TYR:N     | 2.81                     | 0.48              |
| 11:K:353:THR:HG22 | 11:K:355:LEU:H    | 1.79                     | 0.48              |
| 7:i:161:ASP:OD1   | 12:h:270:HIS:NE2  | 2.43                     | 0.48              |
| 9:g:292:SER:HB2   | 9:g:371:ILE:HG12  | 1.96                     | 0.48              |
| 12:h:304:VAL:HG21 | 12:h:401:TYR:CE1  | 2.48                     | 0.48              |
| 3:E:268:TRP:CE3   | 3:E:271:ARG:HD2   | 2.49                     | 0.47              |
| 6:D:436:TYR:N     | 6:D:436:TYR:HD1   | 2.11                     | 0.47              |
| 9:G:273:HIS:CD2   | 9:G:308:THR:HG23  | 2.49                     | 0.47              |
| 9:G:523:TRP:NE1   | 9:G:563:PRO:HB2   | 2.28                     | 0.47              |
| 12:H:12:TYR:HB2   | 12:H:44:ILE:HD12  | 1.95                     | 0.47              |
| 6:d:436:TYR:N     | 6:d:436:TYR:CD1   | 2.81                     | 0.47              |
| 12:h:12:TYR:HB2   | 12:h:44:ILE:HD12  | 1.96                     | 0.47              |
| 1:A:473:VAL:HA    | 1:A:489:THR:HB    | 1.96                     | 0.47              |
| 5:B:255:ASP:OD2   | 4:c:4:LYS:NZ      | 2.47                     | 0.47              |
| 7:I:199:ARG:NH2   | 12:H:209:GLY:O    | 2.48                     | 0.47              |
| 9:G:292:SER:HB2   | 9:G:371:ILE:HG12  | 1.96                     | 0.47              |
| 9:G:374:GLU:OE2   | 9:G:431:ASN:N     | 2.45                     | 0.47              |
| 12:H:189:ILE:HG13 | 12:H:204:LEU:HB2  | 1.96                     | 0.47              |
| 10:J:57:VAL:HG13  | 10:J:109:VAL:HG21 | 1.96                     | 0.47              |
| 12:H:101:GLN:CD   | 12:H:302:PRO:HD3  | 2.39                     | 0.47              |
| 5:b:133:CYS:SG    | 5:b:137:LYS:HB3   | 2.54                     | 0.47              |
| 11:K:303:LYS:O    | 12:H:252:ARG:NH1  | 2.48                     | 0.47              |
| 12:H:418:GLU:O    | 12:H:418:GLU:HG2  | 2.14                     | 0.47              |
| 3:e:40:VAL:HG11   | 3:e:97:ALA:HB2    | 1.96                     | 0.47              |
| 6:d:107:PHE:HD1   | 6:d:121:PHE:CZ    | 2.31                     | 0.47              |
| 9:g:273:HIS:CD2   | 9:g:308:THR:HG23  | 2.49                     | 0.47              |
| 11:m:196:PRO:HG2  | 11:k:298:TYR:HD2  | 1.79                     | 0.47              |
| 6:D:160:ASN:ND2   | 6:D:326:VAL:O     | 2.48                     | 0.47              |
| 6:D:534:HIS:CD2   | 6:D:536:GLY:H     | 2.32                     | 0.47              |
| 12:H:421:MET:HE1  | 12:H:429:LYS:HE2  | 1.95                     | 0.47              |
| 1:a:388:PRO:HB3   | 11:k:5:PHE:CZ     | 2.48                     | 0.47              |
| 4:c:53:SER:HB3    | 4:c:97:ARG:HH11   | 1.80                     | 0.47              |
| 4:c:185:ASP:OD1   | 4:c:186:ARG:N     | 2.46                     | 0.47              |
| 5:b:8:LEU:HD22    | 5:b:13:PRO:HG3    | 1.96                     | 0.47              |
| 7:i:155:LYS:HA    | 7:i:174:GLU:HB2   | 1.97                     | 0.47              |
| 12:h:189:ILE:HG13 | 12:h:204:LEU:HB2  | 1.96                     | 0.47              |
| 3:E:15:ALA:O      | 3:E:19:LYS:HG2    | 2.14                     | 0.47              |
| 3:e:268:TRP:CE3   | 3:e:271:ARG:HD2   | 2.49                     | 0.47              |
| 5:b:189:ILE:HD11  | 5:b:228:ALA:HB2   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:k:303:LYS:O    | 12:h:252:ARG:NH1  | 2.48                     | 0.47              |
| 2:F:48:ASP:OD1    | 2:F:49:MET:N      | 2.48                     | 0.47              |
| 3:E:297:TYR:O     | 3:E:301:GLU:HG2   | 2.15                     | 0.47              |
| 4:C:54:CYS:HA     | 13:C:201:SF4:S3   | 2.55                     | 0.47              |
| 6:D:326:VAL:HG22  | 6:D:327:GLY:H     | 1.79                     | 0.47              |
| 7:I:145:ARG:O     | 7:I:145:ARG:HG2   | 2.15                     | 0.47              |
| 7:I:182:LEU:HD12  | 7:I:209:ALA:HB2   | 1.96                     | 0.47              |
| 12:H:151:VAL:HG21 | 12:H:248:MET:HE3  | 1.97                     | 0.47              |
| 1:a:76:PRO:HB3    | 1:a:80:GLU:OE2    | 2.15                     | 0.47              |
| 1:a:116:ASP:OD1   | 1:a:116:ASP:N     | 2.44                     | 0.47              |
| 6:d:344:GLY:HA3   | 6:d:350:TYR:O     | 2.14                     | 0.47              |
| 6:d:366:GLU:HG2   | 6:d:374:LEU:HD23  | 1.96                     | 0.47              |
| 7:i:199:ARG:NH2   | 12:h:209:GLY:O    | 2.48                     | 0.47              |
| 7:i:203:GLN:N     | 7:i:245:ASP:OD1   | 2.47                     | 0.47              |
| 10:j:57:VAL:HG13  | 10:j:109:VAL:HG21 | 1.96                     | 0.47              |
| 11:k:52:ILE:HG12  | 11:k:73:VAL:HG22  | 1.96                     | 0.47              |
| 12:h:54:ILE:HD11  | 12:h:376:ILE:HG12 | 1.97                     | 0.47              |
| 1:A:380:PRO:HB2   | 11:K:24:LEU:HD12  | 1.97                     | 0.47              |
| 4:C:65:ARG:CZ     | 1:a:492:THR:HG23  | 2.45                     | 0.47              |
| 12:H:214:LEU:HD11 | 12:H:241:ILE:HD11 | 1.96                     | 0.47              |
| 1:a:417:SER:HB2   | 1:a:420:CYS:SG    | 2.55                     | 0.47              |
| 1:a:650:MET:O     | 1:a:654:THR:HG22  | 2.15                     | 0.47              |
| 7:i:101:TRP:CD1   | 7:i:120:ALA:HB3   | 2.50                     | 0.47              |
| 9:g:49:THR:HG21   | 9:g:441:LEU:HD21  | 1.95                     | 0.47              |
| 11:k:131:CYS:HB3  | 13:k:405:SF4:S2   | 2.55                     | 0.47              |
| 12:h:108:MET:HG3  | 12:h:115:LEU:HD13 | 1.97                     | 0.47              |
| 6:D:108:GLN:HG3   | 6:D:401:LEU:HD12  | 1.97                     | 0.47              |
| 11:K:348:ILE:HD13 | 11:K:356:PHE:CE2  | 2.50                     | 0.47              |
| 3:e:100:CYS:HB2   | 3:e:104:ASP:HB2   | 1.97                     | 0.47              |
| 5:b:242:PHE:O     | 5:b:246:GLN:HG3   | 2.15                     | 0.47              |
| 6:d:108:GLN:HG3   | 6:d:401:LEU:HD12  | 1.97                     | 0.47              |
| 6:d:160:ASN:ND2   | 6:d:326:VAL:O     | 2.48                     | 0.47              |
| 6:d:164:ASP:OD2   | 6:d:325:GLY:N     | 2.43                     | 0.47              |
| 9:g:373:LEU:HD13  | 9:g:413:ARG:HD2   | 1.96                     | 0.47              |
| 12:h:151:VAL:HG21 | 12:h:248:MET:HE3  | 1.97                     | 0.47              |
| 6:D:401:LEU:HD23  | 6:D:401:LEU:HA    | 1.65                     | 0.47              |
| 7:I:155:LYS:HA    | 7:I:174:GLU:HB2   | 1.97                     | 0.47              |
| 12:H:119:ALA:O    | 12:H:124:GLY:N    | 2.47                     | 0.47              |
| 7:i:145:ARG:HG2   | 7:i:145:ARG:O     | 2.15                     | 0.47              |
| 5:B:8:LEU:HD22    | 5:B:13:PRO:HG3    | 1.96                     | 0.46              |
| 8:L:101:ILE:HG22  | 8:L:111:ILE:HG23  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:h:214:LEU:HD11 | 12:h:241:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:417:SER:HB2   | 1:A:420:CYS:SG    | 2.55                     | 0.46              |
| 7:I:101:TRP:CD1   | 7:I:120:ALA:HB3   | 2.50                     | 0.46              |
| 11:M:196:PRO:HG2  | 11:K:298:TYR:HD2  | 1.79                     | 0.46              |
| 11:K:131:CYS:HB3  | 13:K:405:SF4:S2   | 2.55                     | 0.46              |
| 8:l:131:TYR:O     | 8:l:132:ASP:C     | 2.58                     | 0.46              |
| 12:h:101:GLN:CD   | 12:h:302:PRO:HD3  | 2.39                     | 0.46              |
| 6:D:396:MET:HE3   | 6:D:396:MET:HB2   | 1.79                     | 0.46              |
| 12:H:108:MET:HG3  | 12:H:115:LEU:HD13 | 1.97                     | 0.46              |
| 6:d:46:GLU:OE1    | 6:d:187:ARG:NH2   | 2.48                     | 0.46              |
| 9:g:497:THR:HG21  | 9:g:500:THR:OG1   | 2.16                     | 0.46              |
| 11:k:353:THR:HG22 | 11:k:355:LEU:H    | 1.79                     | 0.46              |
| 9:G:373:LEU:HD13  | 9:G:413:ARG:HD2   | 1.96                     | 0.46              |
| 6:d:534:HIS:CD2   | 6:d:536:GLY:H     | 2.32                     | 0.46              |
| 8:l:101:ILE:HG22  | 8:l:111:ILE:HG23  | 1.97                     | 0.46              |
| 11:k:41:GLY:C     | 11:k:43:CYS:N     | 2.71                     | 0.46              |
| 1:A:76:PRO:HB3    | 1:A:80:GLU:OE2    | 2.15                     | 0.46              |
| 2:F:77:GLU:HB2    | 2:F:80:TYR:HD2    | 1.80                     | 0.46              |
| 4:C:53:SER:HB3    | 4:C:97:ARG:HH11   | 1.80                     | 0.46              |
| 5:B:43:CYS:SG     | 5:B:82:CYS:HA     | 2.56                     | 0.46              |
| 9:G:88:ILE:CG1    | 9:G:90:GLN:HG3    | 2.46                     | 0.46              |
| 9:g:374:GLU:OE2   | 9:g:431:ASN:N     | 2.45                     | 0.46              |
| 3:E:100:CYS:HB2   | 3:E:104:ASP:HB2   | 1.97                     | 0.46              |
| 4:C:105:THR:O     | 4:C:109:MET:HG2   | 2.16                     | 0.46              |
| 5:B:242:PHE:O     | 5:B:246:GLN:HG3   | 2.15                     | 0.46              |
| 6:D:130:LYS:HB3   | 6:D:375:PRO:HD3   | 1.98                     | 0.46              |
| 9:G:79:PHE:HD2    | 9:G:84:ARG:HD3    | 1.81                     | 0.46              |
| 12:H:365:LYS:NZ   | 12:H:382:ILE:O    | 2.40                     | 0.46              |
| 6:d:99:LYS:HG3    | 6:d:100:HIS:CE1   | 2.51                     | 0.46              |
| 1:A:348:LEU:HD23  | 1:A:511:VAL:HG12  | 1.97                     | 0.46              |
| 3:E:77:THR:HG22   | 3:E:132:SER:OG    | 2.16                     | 0.46              |
| 11:K:276:PHE:CE2  | 11:K:318:VAL:HB   | 2.51                     | 0.46              |
| 3:e:77:THR:HG22   | 3:e:132:SER:OG    | 2.16                     | 0.46              |
| 5:b:43:CYS:SG     | 5:b:82:CYS:HA     | 2.56                     | 0.46              |
| 9:g:79:PHE:HD2    | 9:g:84:ARG:HD3    | 1.81                     | 0.46              |
| 8:L:131:TYR:O     | 8:L:132:ASP:C     | 2.58                     | 0.46              |
| 9:G:497:THR:HG21  | 9:G:500:THR:OG1   | 2.16                     | 0.46              |
| 11:k:42:ILE:HD12  | 11:k:89:PRO:HG2   | 1.98                     | 0.46              |
| 11:k:276:PHE:CE2  | 11:k:318:VAL:HB   | 2.51                     | 0.46              |
| 1:A:474:ALA:HA    | 4:c:49:THR:HG23   | 1.97                     | 0.46              |
| 1:A:600:CYS:O     | 1:A:623:ARG:NH2   | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:180:GLU:HG2   | 3:E:191:ARG:HD3   | 1.98                     | 0.46              |
| 1:a:88:LYS:HE3    | 1:a:94:PRO:HG3    | 1.97                     | 0.46              |
| 1:A:636:CYS:SG    | 1:A:637:GLY:N     | 2.89                     | 0.46              |
| 6:D:89:VAL:HA     | 6:D:422:PHE:HZ    | 1.81                     | 0.46              |
| 9:G:139:PRO:HB2   | 9:G:140:ILE:HG12  | 1.98                     | 0.46              |
| 1:a:380:PRO:HB2   | 11:k:24:LEU:HD12  | 1.97                     | 0.46              |
| 3:e:180:GLU:HG2   | 3:e:191:ARG:HD3   | 1.98                     | 0.46              |
| 3:e:297:TYR:O     | 3:e:301:GLU:HG2   | 2.15                     | 0.46              |
| 4:c:54:CYS:HA     | 13:c:201:SF4:S3   | 2.55                     | 0.46              |
| 9:g:410:GLU:O     | 9:g:414:LYS:HG3   | 2.14                     | 0.46              |
| 1:A:88:LYS:HE3    | 1:A:94:PRO:HG3    | 1.97                     | 0.45              |
| 1:A:650:MET:O     | 1:A:654:THR:HG22  | 2.15                     | 0.45              |
| 6:D:36:VAL:HG21   | 6:D:56:CYS:SG     | 2.56                     | 0.45              |
| 12:H:54:ILE:HD11  | 12:H:376:ILE:HG12 | 1.97                     | 0.45              |
| 4:c:105:THR:O     | 4:c:109:MET:HG2   | 2.16                     | 0.45              |
| 6:d:135:ASP:OD2   | 6:d:139:ARG:HG3   | 2.17                     | 0.45              |
| 6:d:326:VAL:HG22  | 6:d:327:GLY:N     | 2.31                     | 0.45              |
| 7:i:228:VAL:N     | 7:i:239:PHE:O     | 2.45                     | 0.45              |
| 11:k:348:ILE:HD13 | 11:k:356:PHE:CE2  | 2.50                     | 0.45              |
| 6:D:99:LYS:HG3    | 6:D:100:HIS:CE1   | 2.51                     | 0.45              |
| 8:L:113:ASP:OD1   | 8:L:118:LEU:HD12  | 2.16                     | 0.45              |
| 9:G:458:LEU:HD13  | 9:G:462:TYR:HD2   | 1.81                     | 0.45              |
| 11:K:83:VAL:HA    | 11:K:86:ILE:HD12  | 1.99                     | 0.45              |
| 2:f:48:ASP:OD1    | 2:f:49:MET:N      | 2.48                     | 0.45              |
| 5:B:248:GLU:HA    | 5:B:251:GLU:HG2   | 1.98                     | 0.45              |
| 6:D:46:GLU:OE1    | 6:D:187:ARG:NH2   | 2.48                     | 0.45              |
| 6:D:420:LEU:HD23  | 6:D:423:LEU:HB2   | 1.99                     | 0.45              |
| 6:d:36:VAL:HG21   | 6:d:56:CYS:SG     | 2.56                     | 0.45              |
| 9:g:458:LEU:HD13  | 9:g:462:TYR:HD2   | 1.81                     | 0.45              |
| 2:F:88:MET:SD     | 3:E:386:HIS:NE2   | 2.80                     | 0.45              |
| 3:E:59:VAL:HG21   | 3:E:88:LEU:HD21   | 1.99                     | 0.45              |
| 9:G:140:ILE:HD13  | 9:G:516:GLU:HG3   | 1.97                     | 0.45              |
| 5:b:53:ASP:HB3    | 5:b:56:VAL:CG1    | 2.42                     | 0.45              |
| 6:d:117:ASP:OD1   | 6:d:477:ILE:HG23  | 2.16                     | 0.45              |
| 2:F:49:MET:HE1    | 3:E:386:HIS:HE2   | 1.81                     | 0.45              |
| 4:C:4:LYS:NZ      | 5:b:255:ASP:OD2   | 2.49                     | 0.45              |
| 5:B:12:ALA:HB3    | 5:B:13:PRO:HD3    | 1.99                     | 0.45              |
| 6:D:129:PHE:CD2   | 6:D:131:THR:HG23  | 2.42                     | 0.45              |
| 11:K:140:ILE:HD13 | 11:K:244:ILE:HG12 | 1.98                     | 0.45              |
| 1:a:219:MET:HE2   | 1:a:219:MET:HB3   | 1.88                     | 0.45              |
| 3:e:59:VAL:HG21   | 3:e:88:LEU:HD21   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:d:89:VAL:HA     | 6:d:422:PHE:HZ    | 1.81                     | 0.45              |
| 9:g:420:MET:HB2   | 9:g:420:MET:HE3   | 1.82                     | 0.45              |
| 12:h:94:GLY:HA2   | 12:h:299:ILE:CD1  | 2.46                     | 0.45              |
| 3:E:35:LEU:HD23   | 3:E:66:ILE:HD11   | 1.98                     | 0.45              |
| 3:e:141:MET:CE    | 3:e:185:GLY:H     | 2.30                     | 0.45              |
| 1:A:492:THR:HG23  | 4:c:65:ARG:CZ     | 2.46                     | 0.45              |
| 7:I:217:TYR:HE1   | 12:H:210:HIS:NE2  | 2.15                     | 0.45              |
| 11:K:237:LYS:HD3  | 11:K:237:LYS:N    | 2.32                     | 0.45              |
| 5:b:248:GLU:HA    | 5:b:251:GLU:HG2   | 1.98                     | 0.45              |
| 6:d:420:LEU:HD23  | 6:d:423:LEU:HB2   | 1.99                     | 0.45              |
| 9:g:139:PRO:HB2   | 9:g:140:ILE:HG12  | 1.98                     | 0.45              |
| 2:F:49:MET:HG2    | 2:F:89:ILE:HD11   | 1.99                     | 0.45              |
| 9:G:254:LEU:HD23  | 9:G:254:LEU:HA    | 1.82                     | 0.45              |
| 9:g:523:TRP:CH2   | 9:g:525:LYS:HD3   | 2.52                     | 0.45              |
| 6:D:534:HIS:HD2   | 6:D:536:GLY:H     | 1.65                     | 0.45              |
| 7:I:112:ASN:HB3   | 7:I:113:ALA:H     | 1.55                     | 0.45              |
| 2:f:77:GLU:HB2    | 2:f:80:TYR:HD2    | 1.80                     | 0.45              |
| 2:f:95:ASN:OD1    | 2:f:95:ASN:N      | 2.50                     | 0.45              |
| 9:g:88:ILE:CG1    | 9:g:90:GLN:HG3    | 2.46                     | 0.45              |
| 11:m:178:GLY:C    | 11:m:180:CYS:H    | 2.24                     | 0.45              |
| 11:k:83:VAL:HA    | 11:k:86:ILE:HD12  | 1.99                     | 0.45              |
| 11:k:140:ILE:HD13 | 11:k:244:ILE:HG12 | 1.98                     | 0.45              |
| 11:k:162:GLU:O    | 11:k:234:VAL:HG12 | 2.16                     | 0.45              |
| 3:E:141:MET:CE    | 3:E:185:GLY:H     | 2.30                     | 0.45              |
| 9:G:96:MET:HA     | 9:G:96:MET:CE     | 2.47                     | 0.45              |
| 12:H:94:GLY:HA2   | 12:H:299:ILE:CD1  | 2.46                     | 0.45              |
| 1:a:348:LEU:HD23  | 1:a:511:VAL:HG12  | 1.97                     | 0.45              |
| 8:l:113:ASP:OD1   | 8:l:118:LEU:HD12  | 2.16                     | 0.45              |
| 9:g:391:HIS:HA    | 9:g:392:PRO:HA    | 1.76                     | 0.45              |
| 9:g:441:LEU:O     | 9:g:444:ILE:HG22  | 2.17                     | 0.45              |
| 1:A:165:ASP:OD1   | 1:a:575:SER:OG    | 2.35                     | 0.44              |
| 1:A:219:MET:HE2   | 1:A:219:MET:HB3   | 1.87                     | 0.44              |
| 3:E:58:THR:HG22   | 3:E:60:ILE:HG13   | 1.98                     | 0.44              |
| 6:D:117:ASP:OD1   | 6:D:477:ILE:HG23  | 2.16                     | 0.44              |
| 6:D:135:ASP:OD2   | 6:D:139:ARG:HG3   | 2.16                     | 0.44              |
| 10:J:18:GLY:HA3   | 19:H:502:MGD:N19  | 2.33                     | 0.44              |
| 10:J:19:ILE:O     | 10:J:23:ILE:HG12  | 2.18                     | 0.44              |
| 1:a:636:CYS:SG    | 1:a:637:GLY:N     | 2.89                     | 0.44              |
| 3:e:93:ASP:OD1    | 3:e:93:ASP:N      | 2.50                     | 0.44              |
| 6:d:417:LEU:O     | 6:d:420:LEU:HB3   | 2.17                     | 0.44              |
| 7:i:217:TYR:HE1   | 12:h:210:HIS:NE2  | 2.15                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:h:334:VAL:O   | 12:h:338:MET:HG2  | 2.16                     | 0.44              |
| 9:G:174:LEU:HD12 | 9:G:174:LEU:HA    | 1.80                     | 0.44              |
| 11:k:66:ASP:OD1  | 11:k:66:ASP:N     | 2.50                     | 0.44              |
| 11:k:237:LYS:HD3 | 11:k:237:LYS:N    | 2.32                     | 0.44              |
| 1:A:449:SER:HB2  | 1:A:454:TYR:HB3   | 2.00                     | 0.44              |
| 6:D:328:VAL:HG12 | 6:D:330:PRO:HD3   | 2.00                     | 0.44              |
| 6:D:417:LEU:O    | 6:D:420:LEU:HB3   | 2.17                     | 0.44              |
| 12:H:334:VAL:O   | 12:H:338:MET:HG2  | 2.17                     | 0.44              |
| 2:f:49:MET:HG2   | 2:f:89:ILE:HD11   | 1.99                     | 0.44              |
| 3:e:35:LEU:HD23  | 3:e:66:ILE:HD11   | 1.98                     | 0.44              |
| 9:g:3:GLU:N      | 9:g:36:VAL:HG11   | 2.32                     | 0.44              |
| 10:j:18:GLY:HA3  | 19:h:502:MGD:N19  | 2.33                     | 0.44              |
| 10:j:19:ILE:O    | 10:j:23:ILE:HG12  | 2.17                     | 0.44              |
| 12:h:58:ARG:HB2  | 12:h:66:MET:HG2   | 2.00                     | 0.44              |
| 9:G:3:GLU:N      | 9:G:36:VAL:HG11   | 2.32                     | 0.44              |
| 9:G:213:THR:OG1  | 9:G:216:GLU:HG3   | 2.17                     | 0.44              |
| 11:M:178:GLY:C   | 11:M:180:CYS:H    | 2.24                     | 0.44              |
| 11:K:42:ILE:HD12 | 11:K:89:PRO:HG2   | 1.98                     | 0.44              |
| 12:H:58:ARG:HG3  | 12:H:66:MET:SD    | 2.57                     | 0.44              |
| 1:a:600:CYS:O    | 1:a:623:ARG:NH2   | 2.49                     | 0.44              |
| 9:g:140:ILE:HD13 | 9:g:516:GLU:HG3   | 1.97                     | 0.44              |
| 10:j:24:GLY:O    | 10:j:27:SER:OG    | 2.29                     | 0.44              |
| 12:h:322:ASN:N   | 12:h:322:ASN:OD1  | 2.51                     | 0.44              |
| 11:K:162:GLU:O   | 11:K:234:VAL:HG12 | 2.16                     | 0.44              |
| 9:g:508:VAL:HG22 | 9:g:513:ILE:HD13  | 2.00                     | 0.44              |
| 11:k:100:GLU:OE2 | 11:k:100:GLU:N    | 2.51                     | 0.44              |
| 6:D:73:LYS:HD3   | 6:D:78:ILE:CD1    | 2.48                     | 0.44              |
| 11:K:128:CYS:O   | 11:K:129:ASN:HB2  | 2.18                     | 0.44              |
| 12:H:218:PHE:O   | 12:H:222:ILE:HG12 | 2.18                     | 0.44              |
| 3:e:58:THR:HG22  | 3:e:60:ILE:HG13   | 1.98                     | 0.44              |
| 6:d:89:VAL:HA    | 6:d:422:PHE:CZ    | 2.52                     | 0.44              |
| 6:d:130:LYS:HB3  | 6:d:375:PRO:HD3   | 1.98                     | 0.44              |
| 6:d:173:ILE:HD12 | 6:d:173:ILE:H     | 1.83                     | 0.44              |
| 6:d:401:LEU:HD23 | 6:d:401:LEU:HA    | 1.64                     | 0.44              |
| 9:g:213:THR:OG1  | 9:g:216:GLU:HG3   | 2.17                     | 0.44              |
| 1:A:575:SER:OG   | 1:a:165:ASP:OD1   | 2.35                     | 0.44              |
| 2:F:95:ASN:OD1   | 2:F:95:ASN:N      | 2.50                     | 0.44              |
| 3:E:93:ASP:OD1   | 3:E:93:ASP:N      | 2.50                     | 0.44              |
| 5:B:221:ILE:HD11 | 4:c:4:LYS:HD3     | 1.99                     | 0.44              |
| 9:G:14:PRO:HA    | 9:G:442:TYR:OH    | 2.18                     | 0.44              |
| 9:G:308:THR:OG1  | 9:G:384:ARG:O     | 2.21                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:523:TRP:CH2   | 9:G:525:LYS:HD3   | 2.52                     | 0.44              |
| 10:J:56:ARG:HB2   | 10:J:114:VAL:HG21 | 2.00                     | 0.44              |
| 12:H:157:PRO:HD2  | 12:H:196:THR:HG21 | 2.00                     | 0.44              |
| 12:H:293:MET:SD   | 12:H:403:MET:HE1  | 2.58                     | 0.44              |
| 2:f:49:MET:HE1    | 3:e:386:HIS:HE2   | 1.81                     | 0.44              |
| 7:i:112:ASN:HB3   | 7:i:113:ALA:H     | 1.55                     | 0.44              |
| 9:g:14:PRO:HA     | 9:g:442:TYR:OH    | 2.18                     | 0.44              |
| 11:k:128:CYS:O    | 11:k:129:ASN:HB2  | 2.18                     | 0.44              |
| 12:h:119:ALA:O    | 12:h:124:GLY:N    | 2.47                     | 0.44              |
| 1:A:204:THR:N     | 1:A:205:PRO:HD2   | 2.33                     | 0.44              |
| 4:C:124:ASN:HD22  | 5:B:206:GLY:HA3   | 1.83                     | 0.44              |
| 9:G:138:THR:HA    | 9:G:139:PRO:HD3   | 1.89                     | 0.44              |
| 12:H:190:ASP:HB2  | 19:H:502:MGD:H1'  | 1.99                     | 0.44              |
| 12:H:315:CYS:HB3  | 12:H:331:THR:OG1  | 2.18                     | 0.44              |
| 3:e:109:TYR:CD2   | 3:e:381:MET:HE2   | 2.53                     | 0.44              |
| 5:b:150:LYS:HE3   | 5:b:189:ILE:HG21  | 2.00                     | 0.44              |
| 7:i:75:ARG:HE     | 7:i:75:ARG:HB3    | 1.43                     | 0.44              |
| 11:k:153:GLU:HB2  | 11:k:156:ALA:HA   | 2.00                     | 0.44              |
| 12:h:293:MET:SD   | 12:h:403:MET:HE1  | 2.58                     | 0.44              |
| 6:D:528:PRO:HG2   | 6:D:540:LEU:CD2   | 2.48                     | 0.44              |
| 8:L:89:GLU:O      | 8:L:95:PRO:HG3    | 2.18                     | 0.44              |
| 9:G:276:HIS:HB2   | 9:G:279:PHE:HD2   | 1.83                     | 0.44              |
| 9:G:441:LEU:O     | 9:G:444:ILE:HG22  | 2.17                     | 0.44              |
| 9:G:521:THR:O     | 9:G:521:THR:HG23  | 2.18                     | 0.44              |
| 6:D:326:VAL:HG22  | 6:D:327:GLY:N     | 2.31                     | 0.43              |
| 7:I:44:ILE:HD13   | 12:H:86:LYS:HG2   | 2.00                     | 0.43              |
| 12:H:110:ILE:HG22 | 12:H:434:MET:HE2  | 1.99                     | 0.43              |
| 6:d:26:LEU:HD23   | 6:d:36:VAL:HG22   | 1.99                     | 0.43              |
| 6:d:346:TYR:HB2   | 6:d:349:VAL:HG22  | 2.00                     | 0.43              |
| 6:d:528:PRO:HG2   | 6:d:540:LEU:CD2   | 2.47                     | 0.43              |
| 9:g:96:MET:HA     | 9:g:96:MET:CE     | 2.47                     | 0.43              |
| 9:g:223:GLU:HG2   | 9:g:260:TYR:CE2   | 2.53                     | 0.43              |
| 10:j:56:ARG:HB2   | 10:j:114:VAL:HG21 | 2.00                     | 0.43              |
| 11:k:338:ILE:HD12 | 11:k:338:ILE:H    | 1.83                     | 0.43              |
| 5:B:49:PHE:CE2    | 5:B:56:VAL:HG13   | 2.53                     | 0.43              |
| 9:G:99:SER:O      | 9:G:100:ILE:C     | 2.61                     | 0.43              |
| 11:K:100:GLU:N    | 11:K:100:GLU:OE2  | 2.51                     | 0.43              |
| 12:H:142:GLU:OE2  | 12:H:146:ARG:NE   | 2.38                     | 0.43              |
| 5:b:49:PHE:HE2    | 5:b:56:VAL:HG13   | 1.83                     | 0.43              |
| 10:j:7:LEU:HD21   | 10:j:80:CYS:HB2   | 2.00                     | 0.43              |
| 12:h:58:ARG:HG3   | 12:h:66:MET:SD    | 2.57                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:B:53:ASP:HB3   | 5:B:56:VAL:CG1    | 2.42                     | 0.43              |
| 12:H:322:ASN:OD1 | 12:H:322:ASN:N    | 2.51                     | 0.43              |
| 2:f:88:MET:SD    | 3:e:386:HIS:NE2   | 2.80                     | 0.43              |
| 4:c:124:ASN:HD22 | 5:b:206:GLY:HA3   | 1.83                     | 0.43              |
| 5:b:3:GLU:HG2    | 5:b:33:LYS:HB3    | 2.01                     | 0.43              |
| 12:h:218:PHE:O   | 12:h:222:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:76:PRO:O     | 1:A:80:GLU:HG2    | 2.19                     | 0.43              |
| 4:C:4:LYS:HD3    | 5:b:221:ILE:HD11  | 2.01                     | 0.43              |
| 5:B:49:PHE:HE2   | 5:B:56:VAL:HG13   | 1.83                     | 0.43              |
| 6:D:89:VAL:HA    | 6:D:422:PHE:CZ    | 2.53                     | 0.43              |
| 6:D:389:CYS:SG   | 6:D:420:LEU:HD13  | 2.58                     | 0.43              |
| 7:I:253:LYS:CG   | 7:I:254:LYS:H     | 2.29                     | 0.43              |
| 8:L:74:THR:HG21  | 8:L:131:TYR:CZ    | 2.53                     | 0.43              |
| 5:b:12:ALA:HB3   | 5:b:13:PRO:HD3    | 1.98                     | 0.43              |
| 6:d:328:VAL:HG12 | 6:d:330:PRO:HD3   | 2.00                     | 0.43              |
| 6:d:403:PRO:HD2  | 6:d:433:THR:HG21  | 2.01                     | 0.43              |
| 7:i:44:ILE:HD13  | 12:h:86:LYS:HG2   | 2.00                     | 0.43              |
| 7:i:181:VAL:HB   | 7:i:200:VAL:HG13  | 2.00                     | 0.43              |
| 9:g:99:SER:O     | 9:g:100:ILE:C     | 2.61                     | 0.43              |
| 12:h:54:ILE:HG22 | 12:h:388:PRO:HG3  | 2.00                     | 0.43              |
| 6:D:316:LEU:HD23 | 6:D:321:VAL:HG21  | 2.00                     | 0.43              |
| 6:D:346:TYR:HB2  | 6:D:349:VAL:HG22  | 2.00                     | 0.43              |
| 6:D:452:THR:HG22 | 6:D:462:ARG:HD2   | 2.00                     | 0.43              |
| 9:G:223:GLU:HG2  | 9:G:260:TYR:CE2   | 2.53                     | 0.43              |
| 12:H:54:ILE:HG22 | 12:H:388:PRO:HG3  | 2.00                     | 0.43              |
| 12:H:129:ALA:HB1 | 12:H:273:ASP:HB3  | 2.00                     | 0.43              |
| 6:d:348:ASN:OD1  | 6:d:348:ASN:N     | 2.51                     | 0.43              |
| 9:g:76:ASP:HA    | 9:g:84:ARG:NH2    | 2.32                     | 0.43              |
| 9:g:121:ALA:O    | 9:g:146:MET:HB2   | 2.18                     | 0.43              |
| 2:F:32:TYR:HB2   | 2:F:33:PRO:HD2    | 2.01                     | 0.43              |
| 5:B:150:LYS:HE3  | 5:B:189:ILE:HG21  | 2.00                     | 0.43              |
| 7:I:161:ASP:OD1  | 12:H:270:HIS:NE2  | 2.43                     | 0.43              |
| 11:K:338:ILE:H   | 11:K:338:ILE:HD12 | 1.83                     | 0.43              |
| 12:H:4:VAL:HG11  | 12:H:21:ARG:NH1   | 2.34                     | 0.43              |
| 5:b:43:CYS:O     | 5:b:44:PRO:C      | 2.60                     | 0.43              |
| 6:d:73:LYS:HD3   | 6:d:78:ILE:CD1    | 2.48                     | 0.43              |
| 6:d:276:VAL:O    | 6:d:280:ILE:HG12  | 2.19                     | 0.43              |
| 7:i:232:VAL:C    | 7:i:234:GLY:H     | 2.26                     | 0.43              |
| 9:g:79:PHE:CB    | 9:g:84:ARG:HE     | 2.31                     | 0.43              |
| 9:g:237:HIS:HB3  | 9:g:238:GLY:H     | 1.59                     | 0.43              |
| 9:g:281:SER:O    | 9:g:281:SER:OG    | 2.27                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:k:285:CYS:O    | 11:k:287:THR:N    | 2.51                     | 0.43              |
| 12:h:110:ILE:HG22 | 12:h:434:MET:HE2  | 1.99                     | 0.43              |
| 3:E:109:TYR:CD2   | 3:E:381:MET:HE2   | 2.53                     | 0.43              |
| 5:B:43:CYS:O      | 5:B:44:PRO:C      | 2.60                     | 0.43              |
| 6:D:26:LEU:HD23   | 6:D:36:VAL:HG22   | 1.99                     | 0.43              |
| 6:D:348:ASN:OD1   | 6:D:348:ASN:N     | 2.51                     | 0.43              |
| 11:K:285:CYS:O    | 11:K:287:THR:N    | 2.51                     | 0.43              |
| 7:i:253:LYS:CG    | 7:i:254:LYS:H     | 2.29                     | 0.43              |
| 8:l:74:THR:HG21   | 8:l:131:TYR:CZ    | 2.53                     | 0.43              |
| 9:g:521:THR:HG23  | 9:g:521:THR:O     | 2.18                     | 0.43              |
| 10:j:25:LYS:NZ    | 12:h:351:ASP:OD2  | 2.50                     | 0.43              |
| 10:j:86:VAL:O     | 10:j:90:GLN:HG2   | 2.19                     | 0.43              |
| 6:D:16:PRO:HA     | 6:D:335:ASN:HD22  | 1.84                     | 0.43              |
| 7:I:181:VAL:HB    | 7:I:200:VAL:HG13  | 2.00                     | 0.43              |
| 9:G:76:ASP:HA     | 9:G:84:ARG:NH2    | 2.32                     | 0.43              |
| 12:H:80:ARG:O     | 12:H:84:LYS:HG2   | 2.19                     | 0.43              |
| 1:a:200:GLN:HA    | 1:a:200:GLN:HE21  | 1.83                     | 0.43              |
| 1:a:388:PRO:HB3   | 11:k:5:PHE:HZ     | 1.84                     | 0.43              |
| 2:f:101:ARG:HH21  | 2:f:130:LEU:HD21  | 1.84                     | 0.43              |
| 5:b:191:TYR:CE1   | 5:b:194:LYS:HA    | 2.54                     | 0.43              |
| 6:d:16:PRO:HA     | 6:d:335:ASN:HD22  | 1.84                     | 0.43              |
| 6:d:534:HIS:HD2   | 6:d:536:GLY:H     | 1.65                     | 0.43              |
| 7:i:92:SER:HB2    | 7:i:93:ASP:H      | 1.54                     | 0.43              |
| 10:j:12:GLN:HE21  | 19:h:502:MGD:H8   | 1.82                     | 0.43              |
| 10:j:15:VAL:HG23  | 12:h:159:HIS:ND1  | 2.34                     | 0.43              |
| 12:h:190:ASP:HB2  | 19:h:502:MGD:H1'  | 1.99                     | 0.43              |
| 7:I:69:VAL:HG11   | 7:I:73:VAL:HG11   | 2.01                     | 0.43              |
| 9:G:508:VAL:HG22  | 9:G:513:ILE:HD13  | 2.00                     | 0.43              |
| 7:i:264:LEU:HD12  | 7:i:264:LEU:HA    | 1.89                     | 0.43              |
| 12:h:204:LEU:HD11 | 12:h:244:VAL:HG21 | 2.01                     | 0.43              |
| 5:B:8:LEU:HA      | 5:B:8:LEU:HD23    | 1.82                     | 0.43              |
| 6:D:403:PRO:HD2   | 6:D:433:THR:HG21  | 2.01                     | 0.43              |
| 9:G:79:PHE:CB     | 9:G:84:ARG:HE     | 2.31                     | 0.43              |
| 9:G:254:LEU:HB3   | 9:G:300:TYR:CE2   | 2.54                     | 0.43              |
| 9:G:275:THR:O     | 9:G:277:ILE:HG13  | 2.19                     | 0.43              |
| 10:J:7:LEU:HD21   | 10:J:80:CYS:HB2   | 2.00                     | 0.43              |
| 11:K:274:ILE:O    | 11:K:320:LYS:NZ   | 2.45                     | 0.43              |
| 12:H:204:LEU:HD11 | 12:H:244:VAL:HG21 | 2.01                     | 0.43              |
| 12:H:249:LYS:HG2  | 12:H:285:ILE:HD11 | 2.01                     | 0.43              |
| 1:a:76:PRO:O      | 1:a:80:GLU:HG2    | 2.18                     | 0.43              |
| 1:a:449:SER:HB2   | 1:a:454:TYR:HB3   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:i:201:GLY:HA2  | 7:i:204:MET:HE3   | 2.00                     | 0.43              |
| 9:g:411:LYS:HA   | 9:g:414:LYS:HE2   | 2.01                     | 0.43              |
| 11:k:273:GLU:OE2 | 11:k:342:ARG:NH1  | 2.52                     | 0.43              |
| 4:C:178:TYR:OH   | 5:B:106:VAL:HG21  | 2.19                     | 0.42              |
| 5:B:191:TYR:CE1  | 5:B:194:LYS:HA    | 2.54                     | 0.42              |
| 9:G:121:ALA:O    | 9:G:146:MET:HB2   | 2.18                     | 0.42              |
| 9:G:344:ASP:HB3  | 12:H:142:GLU:OE1  | 2.20                     | 0.42              |
| 10:J:12:GLN:HE21 | 19:H:502:MGD:H8   | 1.82                     | 0.42              |
| 12:H:58:ARG:HB2  | 12:H:66:MET:HG2   | 2.00                     | 0.42              |
| 9:g:275:THR:O    | 9:g:277:ILE:HG13  | 2.19                     | 0.42              |
| 12:h:315:CYS:HB3 | 12:h:331:THR:OG1  | 2.18                     | 0.42              |
| 2:F:101:ARG:HH21 | 2:F:130:LEU:HD21  | 1.84                     | 0.42              |
| 7:I:245:ASP:H    | 7:I:250:LYS:NZ    | 2.16                     | 0.42              |
| 10:J:103:GLN:CA  | 12:H:268:ARG:HH22 | 2.32                     | 0.42              |
| 11:K:153:GLU:HB2 | 11:K:156:ALA:HA   | 2.00                     | 0.42              |
| 12:H:87:LYS:HD2  | 12:H:341:GLU:O    | 2.19                     | 0.42              |
| 6:d:316:LEU:HD23 | 6:d:321:VAL:HG21  | 2.00                     | 0.42              |
| 8:l:89:GLU:O     | 8:l:95:PRO:HG3    | 2.18                     | 0.42              |
| 1:A:67:THR:CG2   | 1:A:96:ARG:HH21   | 2.32                     | 0.42              |
| 5:B:8:LEU:HD21   | 5:B:20:GLU:HB2    | 2.00                     | 0.42              |
| 6:D:173:ILE:HD12 | 6:D:173:ILE:H     | 1.83                     | 0.42              |
| 9:G:92:LYS:HG3   | 9:G:93:ARG:HG2    | 2.01                     | 0.42              |
| 9:G:101:PRO:HB3  | 9:G:105:LYS:HD3   | 2.00                     | 0.42              |
| 12:H:395:ASP:HB3 | 12:H:416:PRO:HB3  | 2.01                     | 0.42              |
| 1:a:174:TYR:CE2  | 1:a:217:GLU:HG2   | 2.54                     | 0.42              |
| 2:f:14:CYS:HB3   | 2:f:44:THR:HG23   | 2.01                     | 0.42              |
| 2:f:32:TYR:HB2   | 2:f:33:PRO:HD2    | 2.01                     | 0.42              |
| 3:e:88:LEU:HD13  | 3:e:88:LEU:HA     | 1.87                     | 0.42              |
| 6:d:266:ALA:HB3  | 6:d:270:HIS:NE2   | 2.33                     | 0.42              |
| 6:d:389:CYS:SG   | 6:d:420:LEU:HD13  | 2.58                     | 0.42              |
| 7:i:245:ASP:H    | 7:i:250:LYS:NZ    | 2.16                     | 0.42              |
| 9:g:101:PRO:HB3  | 9:g:105:LYS:HD3   | 2.00                     | 0.42              |
| 9:g:237:HIS:HD2  | 9:g:276:HIS:HE1   | 1.66                     | 0.42              |
| 9:g:276:HIS:HB2  | 9:g:279:PHE:HD2   | 1.83                     | 0.42              |
| 9:g:344:ASP:HB3  | 12:h:142:GLU:OE1  | 2.20                     | 0.42              |
| 11:m:228:LYS:HB2 | 11:m:228:LYS:HE2  | 1.89                     | 0.42              |
| 12:h:129:ALA:HB1 | 12:h:273:ASP:HB3  | 2.00                     | 0.42              |
| 12:h:249:LYS:HG2 | 12:h:285:ILE:HD11 | 2.01                     | 0.42              |
| 8:L:121:GLY:HA2  | 8:L:136:LEU:HD21  | 2.02                     | 0.42              |
| 9:G:411:LYS:HA   | 9:G:414:LYS:HE2   | 2.01                     | 0.42              |
| 1:a:67:THR:CG2   | 1:a:96:ARG:HH21   | 2.32                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:b:84:LYS:HB2   | 5:b:158:HIS:HB3   | 2.01                     | 0.42              |
| 6:d:452:THR:HG22 | 6:d:462:ARG:HD2   | 2.00                     | 0.42              |
| 7:i:219:LEU:HD23 | 7:i:219:LEU:HA    | 1.91                     | 0.42              |
| 9:g:164:LEU:HD21 | 9:g:227:TYR:CG    | 2.55                     | 0.42              |
| 10:j:37:ILE:HD11 | 10:j:57:VAL:HG21  | 2.01                     | 0.42              |
| 10:j:130:VAL:CG1 | 12:h:365:LYS:HG2  | 2.48                     | 0.42              |
| 11:k:45:GLU:O    | 11:k:362:LYS:HD2  | 2.20                     | 0.42              |
| 12:h:157:PRO:HD2 | 12:h:196:THR:HG21 | 2.00                     | 0.42              |
| 12:h:436:GLU:O   | 12:h:438:LYS:HG3  | 2.20                     | 0.42              |
| 1:A:174:TYR:CE2  | 1:A:217:GLU:HG2   | 2.54                     | 0.42              |
| 7:I:232:VAL:C    | 7:I:234:GLY:H     | 2.26                     | 0.42              |
| 8:L:84:PRO:HB3   | 11:K:285:CYS:HB2  | 2.02                     | 0.42              |
| 10:J:130:VAL:CG1 | 12:H:365:LYS:HG2  | 2.48                     | 0.42              |
| 12:H:23:THR:HB   | 12:H:33:GLU:HG2   | 2.01                     | 0.42              |
| 5:b:49:PHE:CE2   | 5:b:56:VAL:HG13   | 2.53                     | 0.42              |
| 11:m:215:CYS:SG  | 11:m:216:ASN:N    | 2.93                     | 0.42              |
| 12:h:365:LYS:NZ  | 12:h:382:ILE:O    | 2.40                     | 0.42              |
| 10:J:101:ALA:O   | 12:H:268:ARG:NH2  | 2.52                     | 0.42              |
| 11:M:215:CYS:SG  | 11:M:216:ASN:N    | 2.93                     | 0.42              |
| 12:H:122:CYS:SG  | 12:H:260:MET:HE1  | 2.60                     | 0.42              |
| 7:i:186:GLU:O    | 7:i:206:LYS:HB3   | 2.20                     | 0.42              |
| 9:g:209:TYR:O    | 9:g:209:TYR:CG    | 2.71                     | 0.42              |
| 1:A:457:PHE:O    | 1:A:461:ILE:HG12  | 2.19                     | 0.42              |
| 5:B:3:GLU:HG2    | 5:B:33:LYS:HB3    | 2.01                     | 0.42              |
| 6:D:276:VAL:O    | 6:D:280:ILE:HG12  | 2.19                     | 0.42              |
| 10:J:37:ILE:HD11 | 10:J:57:VAL:HG21  | 2.01                     | 0.42              |
| 6:d:306:ASP:HB3  | 6:d:557:ILE:HG21  | 2.01                     | 0.42              |
| 6:d:419:LYS:HB3  | 6:d:419:LYS:HE2   | 1.84                     | 0.42              |
| 6:d:493:GLU:O    | 6:d:495:PRO:HD3   | 2.19                     | 0.42              |
| 7:i:69:VAL:HG11  | 7:i:73:VAL:HG11   | 2.01                     | 0.42              |
| 7:i:158:ALA:HB2  | 7:i:173:ILE:HD12  | 2.01                     | 0.42              |
| 7:i:219:LEU:HD23 | 12:h:213:GLU:HG3  | 2.02                     | 0.42              |
| 9:g:101:PRO:HG2  | 9:g:397:PHE:CZ    | 2.55                     | 0.42              |
| 4:C:33:ILE:HG21  | 4:C:71:CYS:SG     | 2.60                     | 0.42              |
| 7:I:158:ALA:HB2  | 7:I:173:ILE:HD12  | 2.01                     | 0.42              |
| 7:I:237:TYR:HB2  | 7:I:239:PHE:CE2   | 2.55                     | 0.42              |
| 8:L:81:VAL:O     | 12:H:173:ARG:NH1  | 2.46                     | 0.42              |
| 9:G:209:TYR:O    | 9:G:209:TYR:CG    | 2.71                     | 0.42              |
| 9:G:262:ALA:HB2  | 9:G:270:GLN:O     | 2.20                     | 0.42              |
| 11:K:273:GLU:OE2 | 11:K:342:ARG:NH1  | 2.52                     | 0.42              |
| 4:c:178:TYR:OH   | 5:b:106:VAL:HG21  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:i:43:LYS:HE2   | 12:h:85:ALA:O     | 2.19                     | 0.42              |
| 7:i:237:TYR:HB3  | 7:i:265:LYS:HZ3   | 1.84                     | 0.42              |
| 8:l:121:GLY:HA2  | 8:l:136:LEU:HD21  | 2.02                     | 0.42              |
| 9:g:254:LEU:HB3  | 9:g:300:TYR:CE2   | 2.54                     | 0.42              |
| 12:h:4:VAL:HG11  | 12:h:21:ARG:NH1   | 2.34                     | 0.42              |
| 12:h:122:CYS:SG  | 12:h:260:MET:HE1  | 2.60                     | 0.42              |
| 3:E:88:LEU:HD13  | 3:E:88:LEU:HA     | 1.87                     | 0.42              |
| 3:E:217:LYS:HE3  | 3:E:217:LYS:HB3   | 1.89                     | 0.42              |
| 5:B:11:ILE:HD12  | 5:B:237:PHE:HD1   | 1.85                     | 0.42              |
| 6:D:493:GLU:O    | 6:D:495:PRO:HD3   | 2.19                     | 0.42              |
| 10:J:15:VAL:HG23 | 12:H:159:HIS:ND1  | 2.34                     | 0.42              |
| 10:J:86:VAL:O    | 10:J:90:GLN:HG2   | 2.19                     | 0.42              |
| 12:H:271:ASN:O   | 12:H:274:ILE:HG22 | 2.20                     | 0.42              |
| 12:H:436:GLU:O   | 12:H:438:LYS:HG3  | 2.20                     | 0.42              |
| 1:a:186:MET:HG2  | 1:a:203:LEU:HD22  | 2.01                     | 0.42              |
| 5:b:8:LEU:HD21   | 5:b:20:GLU:HB2    | 2.00                     | 0.42              |
| 5:b:132:VAL:HG12 | 5:b:133:CYS:N     | 2.35                     | 0.42              |
| 9:g:142:ASP:C    | 9:g:143:GLN:HG3   | 2.45                     | 0.42              |
| 12:h:87:LYS:HD2  | 12:h:341:GLU:O    | 2.20                     | 0.42              |
| 1:A:357:TRP:O    | 1:A:359:TYR:N     | 2.53                     | 0.42              |
| 3:E:46:ILE:HG21  | 3:E:55:ALA:HB1    | 2.02                     | 0.42              |
| 5:B:160:MET:HE3  | 5:B:160:MET:HB3   | 1.67                     | 0.42              |
| 5:B:242:PHE:HB3  | 5:B:261:VAL:HG21  | 2.02                     | 0.42              |
| 7:I:201:GLY:HA2  | 7:I:204:MET:HE3   | 2.00                     | 0.42              |
| 8:L:100:LYS:HZ2  | 8:L:100:LYS:HG2   | 1.74                     | 0.42              |
| 9:G:391:HIS:HA   | 9:G:392:PRO:HA    | 1.76                     | 0.42              |
| 10:J:132:MET:HE1 | 12:H:60:ARG:NH2   | 2.35                     | 0.42              |
| 12:H:317:ASP:HB3 | 12:H:325:HIS:HB3  | 2.02                     | 0.42              |
| 4:c:33:ILE:HG21  | 4:c:71:CYS:SG     | 2.60                     | 0.42              |
| 6:d:132:ASN:ND2  | 6:d:375:PRO:HG2   | 2.35                     | 0.42              |
| 9:g:14:PRO:HG2   | 9:g:446:MET:HA    | 2.02                     | 0.42              |
| 10:j:132:MET:HE1 | 12:h:60:ARG:NH2   | 2.35                     | 0.42              |
| 12:h:80:ARG:O    | 12:h:84:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:8:ARG:H      | 1:A:67:THR:HB     | 1.85                     | 0.41              |
| 6:D:132:ASN:ND2  | 6:D:375:PRO:HG2   | 2.35                     | 0.41              |
| 7:I:219:LEU:HD23 | 12:H:213:GLU:HG3  | 2.02                     | 0.41              |
| 9:G:142:ASP:C    | 9:G:143:GLN:HG3   | 2.45                     | 0.41              |
| 11:K:45:GLU:O    | 11:K:362:LYS:HD2  | 2.20                     | 0.41              |
| 2:f:49:MET:HE3   | 2:f:85:ARG:HG2    | 2.02                     | 0.41              |
| 3:e:243:ILE:HD13 | 3:e:243:ILE:HA    | 1.90                     | 0.41              |
| 3:e:329:MET:HE3  | 3:e:333:ILE:HG13  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:242:PHE:HB3   | 5:b:261:VAL:HG21  | 2.02                     | 0.41              |
| 6:d:151:LEU:HD23  | 6:d:151:LEU:HA    | 1.95                     | 0.41              |
| 7:i:237:TYR:HB2   | 7:i:239:PHE:CE2   | 2.55                     | 0.41              |
| 12:h:23:THR:HB    | 12:h:33:GLU:HG2   | 2.01                     | 0.41              |
| 12:h:347:ASN:HB3  | 12:h:371:THR:HG23 | 2.02                     | 0.41              |
| 12:h:395:ASP:HB3  | 12:h:416:PRO:HB3  | 2.01                     | 0.41              |
| 2:F:14:CYS:HB3    | 2:F:44:THR:HG23   | 2.01                     | 0.41              |
| 2:F:86:MET:HB3    | 2:F:103:PHE:HE2   | 1.85                     | 0.41              |
| 5:B:79:CYS:HB3    | 5:B:82:CYS:HB2    | 2.02                     | 0.41              |
| 5:B:84:LYS:HB2    | 5:B:158:HIS:HB3   | 2.01                     | 0.41              |
| 9:G:116:THR:HG21  | 9:G:472:ASN:CG    | 2.45                     | 0.41              |
| 11:M:197:GLU:HB2  | 11:M:198:ILE:HD12 | 2.02                     | 0.41              |
| 1:a:457:PHE:O     | 1:a:461:ILE:HG12  | 2.19                     | 0.41              |
| 2:f:86:MET:HB3    | 2:f:103:PHE:HE2   | 1.85                     | 0.41              |
| 5:b:11:ILE:HD12   | 5:b:237:PHE:HD1   | 1.85                     | 0.41              |
| 9:g:236:ILE:O     | 9:g:275:THR:HG22  | 2.20                     | 0.41              |
| 12:h:140:LEU:HD13 | 12:h:168:TYR:CD2  | 2.55                     | 0.41              |
| 12:h:165:MET:HA   | 12:h:169:SER:OG   | 2.20                     | 0.41              |
| 12:h:271:ASN:O    | 12:h:274:ILE:HG22 | 2.20                     | 0.41              |
| 12:h:317:ASP:HB3  | 12:h:325:HIS:HB3  | 2.02                     | 0.41              |
| 6:D:306:ASP:HB3   | 6:D:557:ILE:HG21  | 2.01                     | 0.41              |
| 7:I:43:LYS:HE2    | 12:H:85:ALA:O     | 2.19                     | 0.41              |
| 7:I:109:VAL:HB    | 7:I:128:ILE:HG12  | 2.03                     | 0.41              |
| 7:I:134:ASN:HB3   | 7:I:160:ASN:H     | 1.85                     | 0.41              |
| 9:G:101:PRO:HG2   | 9:G:397:PHE:CZ    | 2.55                     | 0.41              |
| 9:G:207:VAL:HG23  | 9:G:212:ILE:O     | 2.20                     | 0.41              |
| 10:J:24:GLY:O     | 10:J:27:SER:OG    | 2.29                     | 0.41              |
| 12:H:347:ASN:HB3  | 12:H:371:THR:HG23 | 2.02                     | 0.41              |
| 7:i:182:LEU:HD23  | 7:i:182:LEU:HA    | 1.86                     | 0.41              |
| 10:j:55:VAL:HG23  | 10:j:113:PRO:HA   | 2.02                     | 0.41              |
| 12:h:58:ARG:HA    | 12:h:68:ASP:HA    | 2.02                     | 0.41              |
| 9:G:14:PRO:HG2    | 9:G:446:MET:HA    | 2.02                     | 0.41              |
| 9:G:236:ILE:O     | 9:G:275:THR:HG22  | 2.20                     | 0.41              |
| 10:J:7:LEU:HD23   | 10:J:7:LEU:O      | 2.21                     | 0.41              |
| 1:a:188:GLN:NE2   | 1:a:279:PHE:O     | 2.54                     | 0.41              |
| 1:a:476:VAL:CG1   | 1:a:485:LEU:HD12  | 2.51                     | 0.41              |
| 6:d:476:ASP:OD1   | 6:d:476:ASP:N     | 2.52                     | 0.41              |
| 6:D:164:ASP:OD2   | 6:D:325:GLY:N     | 2.43                     | 0.41              |
| 7:I:186:GLU:O     | 7:I:206:LYS:HB3   | 2.20                     | 0.41              |
| 10:J:55:VAL:HG12  | 10:J:66:VAL:O     | 2.21                     | 0.41              |
| 1:a:188:GLN:HG2   | 1:a:279:PHE:CE1   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:b:37:LEU:HD12  | 5:b:37:LEU:HA     | 1.84                     | 0.41              |
| 7:i:13:GLU:H     | 7:i:13:GLU:CD     | 2.27                     | 0.41              |
| 9:g:207:VAL:HG23 | 9:g:212:ILE:O     | 2.20                     | 0.41              |
| 12:h:15:CYS:SG   | 12:h:161:HIS:HB3  | 2.60                     | 0.41              |
| 1:A:448:ARG:HG2  | 1:a:448:ARG:HG2   | 2.01                     | 0.41              |
| 7:I:228:VAL:N    | 7:I:239:PHE:O     | 2.45                     | 0.41              |
| 9:G:237:HIS:HD2  | 9:G:276:HIS:HE1   | 1.66                     | 0.41              |
| 11:K:66:ASP:OD1  | 11:K:66:ASP:N     | 2.49                     | 0.41              |
| 12:H:58:ARG:HA   | 12:H:68:ASP:HA    | 2.02                     | 0.41              |
| 3:e:213:ASP:OD1  | 3:e:213:ASP:N     | 2.53                     | 0.41              |
| 7:i:134:ASN:HB3  | 7:i:160:ASN:H     | 1.85                     | 0.41              |
| 9:g:13:ASP:CG    | 9:g:465:LEU:H     | 2.29                     | 0.41              |
| 9:g:347:LEU:HD11 | 9:g:545:ASN:HB3   | 2.03                     | 0.41              |
| 10:j:44:MET:HE1  | 10:j:51:LYS:HA    | 2.02                     | 0.41              |
| 10:j:101:ALA:O   | 12:h:268:ARG:NH2  | 2.53                     | 0.41              |
| 1:A:188:GLN:HG2  | 1:A:279:PHE:CE1   | 2.55                     | 0.41              |
| 1:A:388:PRO:HB3  | 11:K:5:PHE:HZ     | 1.84                     | 0.41              |
| 1:A:426:LYS:HE3  | 1:A:426:LYS:HB3   | 1.67                     | 0.41              |
| 2:F:49:MET:HE3   | 2:F:85:ARG:HG2    | 2.02                     | 0.41              |
| 6:D:361:ASN:O    | 6:D:365:MET:HG2   | 2.21                     | 0.41              |
| 6:D:394:LYS:HA   | 6:D:420:LEU:HD12  | 2.03                     | 0.41              |
| 6:D:458:ARG:HG2  | 6:D:527:TRP:NE1   | 2.35                     | 0.41              |
| 9:G:164:LEU:HD21 | 9:G:227:TYR:CG    | 2.55                     | 0.41              |
| 10:J:25:LYS:NZ   | 12:H:351:ASP:OD2  | 2.50                     | 0.41              |
| 10:J:51:LYS:HB2  | 5:b:296:LEU:HB3   | 2.02                     | 0.41              |
| 11:K:20:GLU:HA   | 11:K:28:ASN:O     | 2.20                     | 0.41              |
| 12:H:165:MET:HA  | 12:H:169:SER:OG   | 2.20                     | 0.41              |
| 1:a:8:ARG:H      | 1:a:67:THR:HB     | 1.85                     | 0.41              |
| 1:a:136:LEU:HD22 | 1:a:652:HIS:CD2   | 2.56                     | 0.41              |
| 1:a:234:PHE:HB2  | 1:a:337:VAL:HG23  | 2.03                     | 0.41              |
| 5:b:44:PRO:HG2   | 5:b:57:TRP:CD1    | 2.56                     | 0.41              |
| 5:b:99:LEU:HD23  | 5:b:99:LEU:HA     | 1.88                     | 0.41              |
| 6:d:9:LYS:HE3    | 6:d:9:LYS:HB3     | 1.77                     | 0.41              |
| 6:d:361:ASN:O    | 6:d:365:MET:HG2   | 2.21                     | 0.41              |
| 9:g:92:LYS:HG3   | 9:g:93:ARG:HG2    | 2.01                     | 0.41              |
| 10:j:103:GLN:CA  | 12:h:268:ARG:HH22 | 2.32                     | 0.41              |
| 11:k:135:CYS:SG  | 11:k:137:ARG:O    | 2.79                     | 0.41              |
| 3:E:254:ARG:HH11 | 3:E:254:ARG:HD3   | 1.75                     | 0.41              |
| 5:B:132:VAL:HG12 | 5:B:133:CYS:N     | 2.35                     | 0.41              |
| 6:D:376:ASP:OD1  | 6:D:376:ASP:C     | 2.64                     | 0.41              |
| 6:D:430:PHE:HE2  | 6:D:435:GLN:HE21  | 1.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:484:PRO:HD2   | 9:G:490:ILE:HD11  | 2.02                     | 0.41              |
| 11:K:46:VAL:O     | 11:K:47:CYS:C     | 2.63                     | 0.41              |
| 12:H:140:LEU:HD13 | 12:H:168:TYR:CD2  | 2.55                     | 0.41              |
| 8:l:84:PRO:HB3    | 11:k:285:CYS:HB2  | 2.02                     | 0.41              |
| 9:g:528:MET:HE2   | 9:g:528:MET:HB3   | 1.85                     | 0.41              |
| 4:C:99:PRO:HG3    | 1:a:472:ARG:CZ    | 2.51                     | 0.41              |
| 5:B:44:PRO:HG2    | 5:B:57:TRP:CD1    | 2.56                     | 0.41              |
| 7:I:15:PHE:CD2    | 12:H:341:GLU:HG3  | 2.56                     | 0.41              |
| 9:G:263:LYS:HE2   | 9:G:263:LYS:HA    | 2.03                     | 0.41              |
| 10:J:55:VAL:HG23  | 10:J:113:PRO:HA   | 2.02                     | 0.41              |
| 10:J:132:MET:HE1  | 12:H:60:ARG:CZ    | 2.51                     | 0.41              |
| 11:M:177:CYS:HB2  | 11:M:179:ILE:HG13 | 2.02                     | 0.41              |
| 12:H:15:CYS:SG    | 12:H:161:HIS:HB3  | 2.60                     | 0.41              |
| 6:d:396:MET:HE3   | 6:d:396:MET:HB2   | 1.79                     | 0.41              |
| 6:d:424:VAL:HG13  | 6:d:439:VAL:HB    | 2.02                     | 0.41              |
| 7:i:15:PHE:HB3    | 7:i:77:LYS:HD3    | 2.03                     | 0.41              |
| 7:i:240:ASP:OD1   | 7:i:240:ASP:N     | 2.46                     | 0.41              |
| 9:g:214:PRO:HA    | 9:g:217:ILE:HG22  | 2.03                     | 0.41              |
| 9:g:254:LEU:HD23  | 9:g:254:LEU:HA    | 1.82                     | 0.41              |
| 11:m:177:CYS:HB2  | 11:m:179:ILE:HG13 | 2.02                     | 0.41              |
| 11:k:20:GLU:HA    | 11:k:28:ASN:O     | 2.20                     | 0.41              |
| 11:k:313:GLU:HG2  | 12:h:179:LYS:NZ   | 2.36                     | 0.41              |
| 1:A:93:ASN:ND2    | 1:A:139:LEU:H     | 2.19                     | 0.41              |
| 1:A:154:GLY:O     | 1:A:159:GLY:HA3   | 2.21                     | 0.41              |
| 5:B:99:LEU:HD23   | 5:B:99:LEU:HA     | 1.88                     | 0.41              |
| 7:I:13:GLU:H      | 7:I:13:GLU:CD     | 2.27                     | 0.41              |
| 7:I:216:LEU:HG    | 7:I:217:TYR:CE2   | 2.56                     | 0.41              |
| 9:G:286:SER:O     | 9:G:290:PHE:HB2   | 2.21                     | 0.41              |
| 10:J:18:GLY:HA3   | 19:H:502:MGD:H191 | 1.86                     | 0.41              |
| 12:H:92:GLY:HA3   | 12:H:348:ILE:O    | 2.21                     | 0.41              |
| 2:f:49:MET:HB3    | 2:f:89:ILE:HD11   | 2.03                     | 0.41              |
| 3:e:46:ILE:HG21   | 3:e:55:ALA:HB1    | 2.02                     | 0.41              |
| 6:d:42:SER:HA     | 6:d:43:PRO:HD2    | 1.93                     | 0.41              |
| 6:d:458:ARG:HG2   | 6:d:527:TRP:NE1   | 2.35                     | 0.41              |
| 7:i:39:ALA:HB2    | 7:i:48:LEU:HD13   | 2.03                     | 0.41              |
| 9:g:107:GLY:HA2   | 9:g:141:LEU:CD1   | 2.51                     | 0.41              |
| 9:g:116:THR:HG21  | 9:g:472:ASN:CG    | 2.46                     | 0.41              |
| 9:g:155:CYS:O     | 9:g:159:ILE:HD13  | 2.21                     | 0.41              |
| 9:g:262:ALA:HB2   | 9:g:270:GLN:O     | 2.20                     | 0.41              |
| 11:k:46:VAL:O     | 11:k:47:CYS:C     | 2.63                     | 0.41              |
| 11:k:274:ILE:O    | 11:k:320:LYS:NZ   | 2.45                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:75:TYR:O     | 2:F:77:GLU:N      | 2.54                     | 0.40              |
| 6:D:42:SER:HA    | 6:D:43:PRO:HD2    | 1.93                     | 0.40              |
| 6:D:424:VAL:HG13 | 6:D:439:VAL:HB    | 2.02                     | 0.40              |
| 9:G:155:CYS:O    | 9:G:159:ILE:HD13  | 2.21                     | 0.40              |
| 3:e:276:MET:HE1  | 3:e:286:MET:HE2   | 2.03                     | 0.40              |
| 6:d:394:LYS:HA   | 6:d:420:LEU:HD12  | 2.03                     | 0.40              |
| 9:g:521:THR:HG22 | 9:g:561:HIS:O     | 2.21                     | 0.40              |
| 10:j:7:LEU:O     | 10:j:7:LEU:HD23   | 2.21                     | 0.40              |
| 10:j:132:MET:HE1 | 12:h:60:ARG:CZ    | 2.51                     | 0.40              |
| 11:k:285:CYS:C   | 11:k:287:THR:H    | 2.29                     | 0.40              |
| 12:h:92:GLY:HA3  | 12:h:348:ILE:O    | 2.21                     | 0.40              |
| 12:h:136:PRO:O   | 12:h:290:ILE:HG22 | 2.21                     | 0.40              |
| 12:h:367:HIS:HB3 | 12:h:368:PRO:HD2  | 2.03                     | 0.40              |
| 1:A:136:LEU:HD22 | 1:A:652:HIS:CD2   | 2.56                     | 0.40              |
| 1:A:188:GLN:NE2  | 1:A:279:PHE:O     | 2.54                     | 0.40              |
| 1:A:476:VAL:CG1  | 1:A:485:LEU:HD12  | 2.51                     | 0.40              |
| 3:E:16:GLU:HG3   | 3:E:67:ILE:HD11   | 2.03                     | 0.40              |
| 9:G:13:ASP:CG    | 9:G:465:LEU:H     | 2.29                     | 0.40              |
| 9:G:521:THR:HG22 | 9:G:561:HIS:O     | 2.21                     | 0.40              |
| 11:K:312:ILE:O   | 11:K:313:GLU:HB2  | 2.22                     | 0.40              |
| 3:e:16:GLU:HG3   | 3:e:67:ILE:HD11   | 2.03                     | 0.40              |
| 6:d:376:ASP:C    | 6:d:376:ASP:OD1   | 2.64                     | 0.40              |
| 7:i:216:LEU:HG   | 7:i:217:TYR:CE2   | 2.56                     | 0.40              |
| 9:g:263:LYS:HE2  | 9:g:263:LYS:HA    | 2.03                     | 0.40              |
| 9:g:500:THR:HB   | 9:g:508:VAL:HB    | 2.03                     | 0.40              |
| 10:j:63:GLU:HG3  | 10:j:64:VAL:N     | 2.35                     | 0.40              |
| 10:j:132:MET:HE2 | 10:j:132:MET:HB3  | 1.88                     | 0.40              |
| 11:m:197:GLU:HB2 | 11:m:198:ILE:HD12 | 2.02                     | 0.40              |
| 1:A:43:ASP:OD1   | 1:A:44:GLN:N      | 2.48                     | 0.40              |
| 3:E:243:ILE:HD13 | 3:E:243:ILE:HA    | 1.90                     | 0.40              |
| 3:E:282:ARG:O    | 3:E:286:MET:HG3   | 2.21                     | 0.40              |
| 3:E:329:MET:HE3  | 3:E:333:ILE:HG13  | 2.02                     | 0.40              |
| 8:L:140:PRO:HA   | 8:L:141:PRO:HD3   | 1.89                     | 0.40              |
| 11:K:313:GLU:HG2 | 12:H:179:LYS:NZ   | 2.36                     | 0.40              |
| 12:H:367:HIS:HB3 | 12:H:368:PRO:HD2  | 2.03                     | 0.40              |
| 12:H:373:ASP:O   | 12:H:388:PRO:HA   | 2.22                     | 0.40              |
| 1:a:431:ILE:HG13 | 1:a:432:MET:N     | 2.36                     | 0.40              |
| 1:a:540:LYS:HA   | 1:a:540:LYS:HD2   | 1.84                     | 0.40              |
| 2:f:75:TYR:O     | 2:f:77:GLU:N      | 2.54                     | 0.40              |
| 2:f:130:LEU:HD23 | 2:f:130:LEU:HA    | 1.76                     | 0.40              |
| 3:e:152:THR:CG2  | 3:e:167:TYR:HB2   | 2.48                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:e:296:CYS:HA    | 6:d:51:PRO:HG3    | 2.03                     | 0.40              |
| 6:d:149:LEU:HD12  | 6:d:149:LEU:HA    | 1.94                     | 0.40              |
| 7:i:7:THR:HG22    | 7:i:70:ASN:HB2    | 2.02                     | 0.40              |
| 7:i:15:PHE:CD2    | 12:h:341:GLU:HG3  | 2.56                     | 0.40              |
| 9:g:484:PRO:HD2   | 9:g:490:ILE:HD11  | 2.02                     | 0.40              |
| 11:k:5:PHE:N      | 11:k:6:PRO:HD2    | 2.36                     | 0.40              |
| 11:k:312:ILE:O    | 11:k:313:GLU:HB2  | 2.22                     | 0.40              |
| 12:h:107:VAL:HG22 | 12:h:431:ALA:HB2  | 2.04                     | 0.40              |
| 14:E:505:FAD:H9   | 14:E:505:FAD:H1'1 | 1.79                     | 0.40              |
| 6:D:476:ASP:OD1   | 6:D:476:ASP:N     | 2.53                     | 0.40              |
| 9:G:65:LYS:NZ     | 9:G:324:ALA:HB2   | 2.36                     | 0.40              |
| 9:G:146:MET:HE2   | 9:G:184:KCX:HB3   | 2.03                     | 0.40              |
| 9:G:347:LEU:HD11  | 9:G:545:ASN:HB3   | 2.03                     | 0.40              |
| 11:K:5:PHE:N      | 11:K:6:PRO:HD2    | 2.36                     | 0.40              |
| 12:H:8:VAL:HG12   | 12:H:9:GLY:N      | 2.36                     | 0.40              |
| 5:b:84:LYS:O      | 5:b:88:GLU:HB3    | 2.22                     | 0.40              |
| 5:b:274:MET:HE2   | 5:b:274:MET:HB3   | 1.98                     | 0.40              |
| 10:j:18:GLY:HA3   | 19:h:502:MGD:H191 | 1.86                     | 0.40              |
| 10:j:73:GLN:NE2   | 12:h:194:THR:HA   | 2.31                     | 0.40              |
| 12:h:57:PRO:HA    | 12:h:388:PRO:HD3  | 2.03                     | 0.40              |
| 12:h:347:ASN:HB3  | 12:h:371:THR:HA   | 2.03                     | 0.40              |
| 3:E:276:MET:HE1   | 3:E:286:MET:HE2   | 2.04                     | 0.40              |
| 3:E:296:CYS:HA    | 6:D:51:PRO:HG3    | 2.04                     | 0.40              |
| 7:I:7:THR:HG22    | 7:I:70:ASN:HB2    | 2.02                     | 0.40              |
| 7:I:117:LEU:HD11  | 7:I:126:ILE:HG21  | 2.04                     | 0.40              |
| 12:H:136:PRO:O    | 12:H:290:ILE:HG22 | 2.21                     | 0.40              |
| 5:b:18:GLY:HA3    | 5:b:279:LEU:O     | 2.21                     | 0.40              |
| 6:d:205:ARG:HG3   | 6:d:207:THR:HG23  | 2.03                     | 0.40              |
| 6:d:274:LEU:HD12  | 6:d:274:LEU:HA    | 1.95                     | 0.40              |
| 12:h:8:VAL:HG12   | 12:h:9:GLY:N      | 2.36                     | 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     | 660/671 (98%)   | 626 (95%)  | 33 (5%)  | 1 (0%)   | 43          | 76  |
| 1   | a     | 660/671 (98%)   | 627 (95%)  | 32 (5%)  | 1 (0%)   | 43          | 76  |
| 2   | F     | 135/140 (96%)   | 126 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 2   | f     | 135/140 (96%)   | 126 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 3   | E     | 409/414 (99%)   | 389 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 3   | e     | 409/414 (99%)   | 389 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 4   | C     | 187/191 (98%)   | 179 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 4   | c     | 187/191 (98%)   | 179 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 5   | B     | 294/296 (99%)   | 279 (95%)  | 15 (5%)  | 0        | 100         | 100 |
| 5   | b     | 294/296 (99%)   | 279 (95%)  | 15 (5%)  | 0        | 100         | 100 |
| 6   | D     | 545/686 (79%)   | 506 (93%)  | 39 (7%)  | 0        | 100         | 100 |
| 6   | d     | 545/686 (79%)   | 506 (93%)  | 39 (7%)  | 0        | 100         | 100 |
| 7   | I     | 262/266 (98%)   | 226 (86%)  | 35 (13%) | 1 (0%)   | 30          | 65  |
| 7   | i     | 262/266 (98%)   | 226 (86%)  | 35 (13%) | 1 (0%)   | 30          | 65  |
| 8   | L     | 77/146 (53%)    | 72 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 8   | l     | 77/146 (53%)    | 72 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 9   | G     | 565/571 (99%)   | 514 (91%)  | 49 (9%)  | 2 (0%)   | 30          | 65  |
| 9   | g     | 565/571 (99%)   | 514 (91%)  | 49 (9%)  | 2 (0%)   | 30          | 65  |
| 10  | J     | 129/137 (94%)   | 118 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 10  | j     | 129/137 (94%)   | 118 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 11  | K     | 317/388 (82%)   | 276 (87%)  | 40 (13%) | 1 (0%)   | 36          | 70  |
| 11  | M     | 63/388 (16%)    | 55 (87%)   | 7 (11%)  | 1 (2%)   | 7           | 34  |
| 11  | k     | 317/388 (82%)   | 276 (87%)  | 40 (13%) | 1 (0%)   | 36          | 70  |
| 11  | m     | 63/388 (16%)    | 55 (87%)   | 7 (11%)  | 1 (2%)   | 7           | 34  |
| 12  | H     | 436/443 (98%)   | 390 (89%)  | 46 (11%) | 0        | 100         | 100 |
| 12  | h     | 436/443 (98%)   | 390 (89%)  | 46 (11%) | 0        | 100         | 100 |
| All | All   | 8158/9474 (86%) | 7513 (92%) | 633 (8%) | 12 (0%)  | 49          | 80  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | G     | 276 | HIS  |
| 9   | g     | 276 | HIS  |
| 1   | A     | 446 | ASP  |
| 11  | K     | 42  | ILE  |
| 1   | a     | 446 | ASP  |
| 11  | k     | 42  | ILE  |
| 7   | I     | 92  | SER  |
| 9   | G     | 348 | GLU  |
| 7   | i     | 92  | SER  |
| 9   | g     | 348 | GLU  |
| 11  | M     | 179 | ILE  |
| 11  | m     | 179 | ILE  |

### 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     | 536/543 (99%)  | 526 (98%)  | 10 (2%)  | 50          | 76  |
| 1   | a     | 536/543 (99%)  | 524 (98%)  | 12 (2%)  | 45          | 74  |
| 2   | F     | 112/114 (98%)  | 108 (96%)  | 4 (4%)   | 31          | 65  |
| 2   | f     | 112/114 (98%)  | 108 (96%)  | 4 (4%)   | 31          | 65  |
| 3   | E     | 338/341 (99%)  | 327 (97%)  | 11 (3%)  | 33          | 67  |
| 3   | e     | 338/341 (99%)  | 327 (97%)  | 11 (3%)  | 33          | 67  |
| 4   | C     | 168/170 (99%)  | 168 (100%) | 0        | 100         | 100 |
| 4   | c     | 168/170 (99%)  | 168 (100%) | 0        | 100         | 100 |
| 5   | B     | 245/245 (100%) | 239 (98%)  | 6 (2%)   | 43          | 73  |
| 5   | b     | 245/245 (100%) | 239 (98%)  | 6 (2%)   | 43          | 73  |
| 6   | D     | 454/571 (80%)  | 438 (96%)  | 16 (4%)  | 32          | 65  |
| 6   | d     | 454/571 (80%)  | 438 (96%)  | 16 (4%)  | 32          | 65  |
| 7   | I     | 202/204 (99%)  | 187 (93%)  | 15 (7%)  | 13          | 42  |
| 7   | i     | 202/204 (99%)  | 187 (93%)  | 15 (7%)  | 13          | 42  |
| 8   | L     | 67/128 (52%)   | 59 (88%)   | 8 (12%)  | 5           | 22  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 8   | l     | 67/128 (52%)    | 59 (88%)   | 8 (12%)  | 5           | 22 |
| 9   | G     | 472/474 (100%)  | 463 (98%)  | 9 (2%)   | 50          | 76 |
| 9   | g     | 472/474 (100%)  | 463 (98%)  | 9 (2%)   | 50          | 76 |
| 10  | J     | 111/116 (96%)   | 110 (99%)  | 1 (1%)   | 70          | 85 |
| 10  | j     | 111/116 (96%)   | 110 (99%)  | 1 (1%)   | 70          | 85 |
| 11  | K     | 275/332 (83%)   | 260 (94%)  | 15 (6%)  | 19          | 53 |
| 11  | M     | 55/332 (17%)    | 44 (80%)   | 11 (20%) | 1           | 7  |
| 11  | k     | 275/332 (83%)   | 260 (94%)  | 15 (6%)  | 19          | 53 |
| 11  | m     | 55/332 (17%)    | 44 (80%)   | 11 (20%) | 1           | 7  |
| 12  | H     | 370/373 (99%)   | 360 (97%)  | 10 (3%)  | 39          | 71 |
| 12  | h     | 370/373 (99%)   | 360 (97%)  | 10 (3%)  | 39          | 71 |
| All | All   | 6810/7886 (86%) | 6576 (97%) | 234 (3%) | 33          | 66 |

All (234) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 198 | CYS  |
| 1   | A     | 199 | SER  |
| 1   | A     | 204 | THR  |
| 1   | A     | 405 | SER  |
| 1   | A     | 420 | CYS  |
| 1   | A     | 423 | TYR  |
| 1   | A     | 426 | LYS  |
| 1   | A     | 520 | LEU  |
| 1   | A     | 561 | LYS  |
| 1   | A     | 562 | ASP  |
| 2   | F     | 42  | MET  |
| 2   | F     | 95  | ASN  |
| 2   | F     | 98  | LEU  |
| 2   | F     | 101 | ARG  |
| 3   | E     | 28  | THR  |
| 3   | E     | 53  | TYR  |
| 3   | E     | 72  | SER  |
| 3   | E     | 88  | LEU  |
| 3   | E     | 99  | THR  |
| 3   | E     | 160 | LYS  |
| 3   | E     | 207 | ASN  |
| 3   | E     | 278 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 280 | LYS  |
| 3   | E     | 281 | ASP  |
| 3   | E     | 284 | LYS  |
| 5   | B     | 160 | MET  |
| 5   | B     | 178 | GLU  |
| 5   | B     | 179 | GLU  |
| 5   | B     | 218 | GLU  |
| 5   | B     | 219 | LYS  |
| 5   | B     | 233 | GLU  |
| 6   | D     | 130 | LYS  |
| 6   | D     | 132 | ASN  |
| 6   | D     | 169 | ASP  |
| 6   | D     | 230 | SER  |
| 6   | D     | 258 | LYS  |
| 6   | D     | 259 | THR  |
| 6   | D     | 305 | THR  |
| 6   | D     | 357 | GLU  |
| 6   | D     | 399 | LEU  |
| 6   | D     | 436 | TYR  |
| 6   | D     | 476 | ASP  |
| 6   | D     | 527 | TRP  |
| 6   | D     | 531 | THR  |
| 6   | D     | 547 | THR  |
| 6   | D     | 549 | ASP  |
| 6   | D     | 553 | ASN  |
| 7   | I     | 16  | LEU  |
| 7   | I     | 73  | VAL  |
| 7   | I     | 75  | ARG  |
| 7   | I     | 76  | MET  |
| 7   | I     | 77  | LYS  |
| 7   | I     | 81  | GLN  |
| 7   | I     | 83  | MET  |
| 7   | I     | 90  | ILE  |
| 7   | I     | 92  | SER  |
| 7   | I     | 95  | ASP  |
| 7   | I     | 102 | MET  |
| 7   | I     | 115 | SER  |
| 7   | I     | 121 | MET  |
| 7   | I     | 170 | THR  |
| 7   | I     | 173 | ILE  |
| 8   | L     | 66  | VAL  |
| 8   | L     | 100 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L     | 101 | ILE  |
| 8   | L     | 103 | LYS  |
| 8   | L     | 124 | ILE  |
| 8   | L     | 131 | TYR  |
| 8   | L     | 132 | ASP  |
| 8   | L     | 133 | VAL  |
| 9   | G     | 96  | MET  |
| 9   | G     | 134 | GLU  |
| 9   | G     | 138 | THR  |
| 9   | G     | 140 | ILE  |
| 9   | G     | 156 | PHE  |
| 9   | G     | 345 | VAL  |
| 9   | G     | 346 | GLU  |
| 9   | G     | 348 | GLU  |
| 9   | G     | 349 | THR  |
| 10  | J     | 63  | GLU  |
| 11  | M     | 169 | VAL  |
| 11  | M     | 171 | ASP  |
| 11  | M     | 172 | GLU  |
| 11  | M     | 173 | LYS  |
| 11  | M     | 175 | THR  |
| 11  | M     | 177 | CYS  |
| 11  | M     | 179 | ILE  |
| 11  | M     | 187 | ILE  |
| 11  | M     | 215 | CYS  |
| 11  | M     | 217 | VAL  |
| 11  | M     | 227 | ILE  |
| 11  | K     | 36  | ILE  |
| 11  | K     | 40  | CYS  |
| 11  | K     | 42  | ILE  |
| 11  | K     | 48  | PRO  |
| 11  | K     | 81  | CYS  |
| 11  | K     | 90  | PHE  |
| 11  | K     | 126 | VAL  |
| 11  | K     | 128 | CYS  |
| 11  | K     | 137 | ARG  |
| 11  | K     | 140 | ILE  |
| 11  | K     | 157 | LYS  |
| 11  | K     | 257 | ILE  |
| 11  | K     | 261 | THR  |
| 11  | K     | 264 | ILE  |
| 11  | K     | 266 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | H     | 95  | SER  |
| 12  | H     | 96  | THR  |
| 12  | H     | 126 | SER  |
| 12  | H     | 220 | MET  |
| 12  | H     | 260 | MET  |
| 12  | H     | 297 | TYR  |
| 12  | H     | 308 | TRP  |
| 12  | H     | 408 | ILE  |
| 12  | H     | 423 | ASP  |
| 12  | H     | 424 | GLU  |
| 1   | a     | 197 | ASP  |
| 1   | a     | 198 | CYS  |
| 1   | a     | 199 | SER  |
| 1   | a     | 200 | GLN  |
| 1   | a     | 204 | THR  |
| 1   | a     | 405 | SER  |
| 1   | a     | 420 | CYS  |
| 1   | a     | 423 | TYR  |
| 1   | a     | 426 | LYS  |
| 1   | a     | 520 | LEU  |
| 1   | a     | 561 | LYS  |
| 1   | a     | 562 | ASP  |
| 2   | f     | 42  | MET  |
| 2   | f     | 95  | ASN  |
| 2   | f     | 98  | LEU  |
| 2   | f     | 101 | ARG  |
| 3   | e     | 28  | THR  |
| 3   | e     | 53  | TYR  |
| 3   | e     | 72  | SER  |
| 3   | e     | 88  | LEU  |
| 3   | e     | 99  | THR  |
| 3   | e     | 160 | LYS  |
| 3   | e     | 207 | ASN  |
| 3   | e     | 278 | LYS  |
| 3   | e     | 280 | LYS  |
| 3   | e     | 281 | ASP  |
| 3   | e     | 284 | LYS  |
| 5   | b     | 160 | MET  |
| 5   | b     | 178 | GLU  |
| 5   | b     | 179 | GLU  |
| 5   | b     | 218 | GLU  |
| 5   | b     | 219 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | b     | 233 | GLU  |
| 6   | d     | 130 | LYS  |
| 6   | d     | 132 | ASN  |
| 6   | d     | 169 | ASP  |
| 6   | d     | 230 | SER  |
| 6   | d     | 258 | LYS  |
| 6   | d     | 259 | THR  |
| 6   | d     | 305 | THR  |
| 6   | d     | 357 | GLU  |
| 6   | d     | 399 | LEU  |
| 6   | d     | 436 | TYR  |
| 6   | d     | 476 | ASP  |
| 6   | d     | 527 | TRP  |
| 6   | d     | 531 | THR  |
| 6   | d     | 547 | THR  |
| 6   | d     | 549 | ASP  |
| 6   | d     | 553 | ASN  |
| 7   | i     | 16  | LEU  |
| 7   | i     | 73  | VAL  |
| 7   | i     | 75  | ARG  |
| 7   | i     | 76  | MET  |
| 7   | i     | 77  | LYS  |
| 7   | i     | 81  | GLN  |
| 7   | i     | 83  | MET  |
| 7   | i     | 90  | ILE  |
| 7   | i     | 92  | SER  |
| 7   | i     | 95  | ASP  |
| 7   | i     | 102 | MET  |
| 7   | i     | 115 | SER  |
| 7   | i     | 121 | MET  |
| 7   | i     | 170 | THR  |
| 7   | i     | 173 | ILE  |
| 8   | l     | 66  | VAL  |
| 8   | l     | 100 | LYS  |
| 8   | l     | 101 | ILE  |
| 8   | l     | 103 | LYS  |
| 8   | l     | 124 | ILE  |
| 8   | l     | 131 | TYR  |
| 8   | l     | 132 | ASP  |
| 8   | l     | 133 | VAL  |
| 9   | g     | 96  | MET  |
| 9   | g     | 134 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | g     | 138 | THR  |
| 9   | g     | 140 | ILE  |
| 9   | g     | 156 | PHE  |
| 9   | g     | 345 | VAL  |
| 9   | g     | 346 | GLU  |
| 9   | g     | 348 | GLU  |
| 9   | g     | 349 | THR  |
| 10  | j     | 63  | GLU  |
| 11  | m     | 169 | VAL  |
| 11  | m     | 171 | ASP  |
| 11  | m     | 172 | GLU  |
| 11  | m     | 173 | LYS  |
| 11  | m     | 175 | THR  |
| 11  | m     | 177 | CYS  |
| 11  | m     | 179 | ILE  |
| 11  | m     | 187 | ILE  |
| 11  | m     | 215 | CYS  |
| 11  | m     | 217 | VAL  |
| 11  | m     | 227 | ILE  |
| 11  | k     | 36  | ILE  |
| 11  | k     | 40  | CYS  |
| 11  | k     | 42  | ILE  |
| 11  | k     | 48  | PRO  |
| 11  | k     | 81  | CYS  |
| 11  | k     | 90  | PHE  |
| 11  | k     | 126 | VAL  |
| 11  | k     | 128 | CYS  |
| 11  | k     | 137 | ARG  |
| 11  | k     | 140 | ILE  |
| 11  | k     | 157 | LYS  |
| 11  | k     | 257 | ILE  |
| 11  | k     | 261 | THR  |
| 11  | k     | 264 | ILE  |
| 11  | k     | 266 | VAL  |
| 12  | h     | 95  | SER  |
| 12  | h     | 96  | THR  |
| 12  | h     | 126 | SER  |
| 12  | h     | 220 | MET  |
| 12  | h     | 260 | MET  |
| 12  | h     | 297 | TYR  |
| 12  | h     | 308 | TRP  |
| 12  | h     | 408 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | h     | 423 | ASP  |
| 12  | h     | 424 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 200 | GLN  |
| 1   | A     | 361 | GLN  |
| 1   | A     | 486 | HIS  |
| 1   | A     | 512 | GLN  |
| 1   | A     | 661 | GLN  |
| 2   | F     | 31  | GLN  |
| 3   | E     | 62  | ASN  |
| 3   | E     | 118 | ASN  |
| 4   | C     | 21  | HIS  |
| 5   | B     | 14  | ASN  |
| 5   | B     | 136 | GLN  |
| 5   | B     | 173 | ASN  |
| 5   | B     | 190 | GLN  |
| 5   | B     | 196 | GLN  |
| 6   | D     | 59  | HIS  |
| 6   | D     | 224 | HIS  |
| 6   | D     | 338 | GLN  |
| 6   | D     | 412 | HIS  |
| 6   | D     | 416 | GLN  |
| 6   | D     | 534 | HIS  |
| 7   | I     | 70  | ASN  |
| 9   | G     | 152 | ASN  |
| 9   | G     | 270 | GLN  |
| 9   | G     | 273 | HIS  |
| 9   | G     | 274 | ASN  |
| 9   | G     | 545 | ASN  |
| 10  | J     | 54  | ASN  |
| 10  | J     | 73  | GLN  |
| 11  | K     | 21  | GLN  |
| 11  | K     | 28  | ASN  |
| 12  | H     | 145 | ASN  |
| 12  | H     | 325 | HIS  |
| 12  | H     | 367 | HIS  |
| 1   | a     | 200 | GLN  |
| 1   | a     | 361 | GLN  |
| 1   | a     | 486 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 661 | GLN  |
| 2   | f     | 31  | GLN  |
| 3   | e     | 62  | ASN  |
| 3   | e     | 118 | ASN  |
| 3   | e     | 128 | ASN  |
| 4   | c     | 21  | HIS  |
| 5   | b     | 14  | ASN  |
| 5   | b     | 136 | GLN  |
| 5   | b     | 190 | GLN  |
| 5   | b     | 196 | GLN  |
| 6   | d     | 59  | HIS  |
| 6   | d     | 224 | HIS  |
| 6   | d     | 338 | GLN  |
| 6   | d     | 412 | HIS  |
| 6   | d     | 416 | GLN  |
| 6   | d     | 534 | HIS  |
| 7   | i     | 70  | ASN  |
| 9   | g     | 152 | ASN  |
| 9   | g     | 270 | GLN  |
| 9   | g     | 273 | HIS  |
| 9   | g     | 274 | ASN  |
| 9   | g     | 545 | ASN  |
| 10  | j     | 54  | ASN  |
| 10  | j     | 73  | GLN  |
| 11  | k     | 21  | GLN  |
| 11  | k     | 28  | ASN  |
| 11  | k     | 243 | ASN  |
| 12  | h     | 145 | ASN  |
| 12  | h     | 325 | HIS  |
| 12  | h     | 386 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | KCX  | g     | 184 | 17,9 | 10,11,12     | 0.36 | 0           | 6,12,14     | 0.45 | 0           |
| 9   | KCX  | G     | 184 | 17,9 | 10,11,12     | 0.36 | 0           | 6,12,14     | 0.46 | 0           |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 9   | KCX  | g     | 184 | 17,9 | -       | 3/9/10/12 | -     |
| 9   | KCX  | G     | 184 | 17,9 | -       | 3/9/10/12 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 9   | G     | 184 | KCX  | OQ1-CX-NZ-CE |
| 9   | g     | 184 | KCX  | OQ1-CX-NZ-CE |
| 9   | G     | 184 | KCX  | OQ2-CX-NZ-CE |
| 9   | g     | 184 | KCX  | OQ2-CX-NZ-CE |
| 9   | G     | 184 | KCX  | N-CA-CB-CG   |
| 9   | g     | 184 | KCX  | N-CA-CB-CG   |

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | g     | 184 | KCX  | 1       | 0            |
| 9   | G     | 184 | KCX  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 6 are monoatomic - leaving 62 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 |
| 13  | SF4  | A     | 706 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | C     | 201 | 4    | 0,12,12      | -    | -        | -           |      |          |
| 16  | 9S8  | B     | 302 | 5    | 4,10,10      | 6.77 | 2 (50%)  | -           |      |          |
| 16  | 9S8  | b     | 302 | 5    | 4,10,10      | 6.79 | 2 (50%)  | -           |      |          |
| 19  | MGD  | h     | 503 | 18   | 47,52,52     | 4.89 | 29 (61%) | 58,81,81    | 2.02 | 16 (27%) |
| 13  | SF4  | a     | 706 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 14  | FAD  | E     | 505 | -    | 58,58,58     | 1.19 | 3 (5%)   | 85,89,89    | 0.43 | 0        |
| 13  | SF4  | M     | 402 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | e     | 502 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | E     | 504 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | a     | 705 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | D     | 701 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | h     | 504 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | L     | 202 | 8    | 0,12,12      | -    | -        | -           |      |          |
| 15  | FES  | F     | 201 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 13  | SF4  | A     | 703 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | A     | 705 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 401 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | E     | 501 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 403 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 15  | FES  | f     | 201 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 13  | SF4  | K     | 404 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 404 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 14  | FAD  | a     | 702 | -    | 58,58,58     | 0.84 | 3 (5%)   | 85,89,89    | 0.44 | 0        |
| 13  | SF4  | M     | 401 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 406 | 11   | 0,12,12      | -    | -        | -           |      |          |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | FAD  | e     | 505 | -    | 58,58,58     | 1.19 | 3 (5%)   | 85,89,89    | 0.43 | 0        |
| 13  | SF4  | e     | 503 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | d     | 701 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 16  | 9S8  | b     | 301 | 5    | 4,10,10      | 6.83 | 2 (50%)  | -           |      |          |
| 19  | MGD  | H     | 502 | 18   | 47,52,52     | 4.84 | 27 (57%) | 58,81,81    | 2.10 | 15 (25%) |
| 13  | SF4  | e     | 504 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | e     | 501 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | c     | 201 | 4    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | K     | 405 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | K     | 403 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | K     | 402 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 16  | 9S8  | B     | 301 | 5    | 4,10,10      | 6.85 | 2 (50%)  | -           |      |          |
| 13  | SF4  | K     | 406 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | l     | 201 | 8    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | l     | 202 | 8    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | A     | 707 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | E     | 502 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | H     | 504 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 19  | MGD  | H     | 503 | 18   | 47,52,52     | 4.89 | 29 (61%) | 58,81,81    | 2.02 | 17 (29%) |
| 13  | SF4  | a     | 704 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | c     | 202 | 4    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | a     | 707 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | K     | 401 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | a     | 703 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | m     | 401 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 14  | FAD  | A     | 702 | -    | 58,58,58     | 0.84 | 3 (5%)   | 85,89,89    | 0.44 | 0        |
| 13  | SF4  | L     | 201 | 8    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | C     | 202 | 4    | 0,12,12      | -    | -        | -           |      |          |
| 19  | MGD  | h     | 502 | 18   | 47,52,52     | 4.83 | 27 (57%) | 58,81,81    | 2.10 | 15 (25%) |
| 13  | SF4  | E     | 503 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 405 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | A     | 704 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | A     | 701 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | a     | 701 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | k     | 402 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 13  | SF4  | m     | 402 | 11   | 0,12,12      | -    | -        | -           |      |          |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 13  | SF4  | A     | 706 | 1    | -       | -           | 0/6/5/5 |
| 13  | SF4  | C     | 201 | 4    | -       | -           | 0/6/5/5 |
| 16  | 9S8  | B     | 302 | 5    | -       | -           | 0/3/3/3 |
| 16  | 9S8  | b     | 302 | 5    | -       | -           | 0/3/3/3 |
| 19  | MGD  | h     | 503 | 18   | -       | 8/22/66/66  | 0/6/6/6 |
| 13  | SF4  | a     | 706 | 1    | -       | -           | 0/6/5/5 |
| 14  | FAD  | E     | 505 | -    | -       | 13/34/50/50 | 0/6/6/6 |
| 13  | SF4  | M     | 402 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | e     | 502 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | E     | 504 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | a     | 705 | 1    | -       | -           | 0/6/5/5 |
| 13  | SF4  | D     | 701 | 6    | -       | -           | 0/6/5/5 |
| 13  | SF4  | h     | 504 | 12   | -       | -           | 0/6/5/5 |
| 13  | SF4  | L     | 202 | 8    | -       | -           | 0/6/5/5 |
| 15  | FES  | F     | 201 | 2    | -       | -           | 0/1/1/1 |
| 13  | SF4  | A     | 703 | 1    | -       | -           | 0/6/5/5 |
| 13  | SF4  | A     | 705 | 1    | -       | -           | 0/6/5/5 |
| 13  | SF4  | k     | 401 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | E     | 501 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | k     | 403 | 11   | -       | -           | 0/6/5/5 |
| 15  | FES  | f     | 201 | 2    | -       | -           | 0/1/1/1 |
| 13  | SF4  | K     | 404 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | k     | 404 | 11   | -       | -           | 0/6/5/5 |
| 14  | FAD  | a     | 702 | -    | -       | 1/34/50/50  | 0/6/6/6 |
| 13  | SF4  | M     | 401 | 11   | -       | -           | 0/6/5/5 |
| 19  | MGD  | H     | 502 | 18   | -       | 8/22/66/66  | 0/6/6/6 |
| 14  | FAD  | e     | 505 | -    | -       | 13/34/50/50 | 0/6/6/6 |
| 13  | SF4  | e     | 503 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | d     | 701 | 6    | -       | -           | 0/6/5/5 |
| 13  | SF4  | k     | 406 | 11   | -       | -           | 0/6/5/5 |
| 16  | 9S8  | b     | 301 | 5    | -       | -           | 0/3/3/3 |
| 13  | SF4  | e     | 504 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | e     | 501 | 3    | -       | -           | 0/6/5/5 |
| 13  | SF4  | c     | 201 | 4    | -       | -           | 0/6/5/5 |
| 13  | SF4  | K     | 405 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | K     | 403 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | K     | 402 | 11   | -       | -           | 0/6/5/5 |
| 16  | 9S8  | B     | 301 | 5    | -       | -           | 0/3/3/3 |
| 13  | SF4  | K     | 406 | 11   | -       | -           | 0/6/5/5 |
| 13  | SF4  | l     | 201 | 8    | -       | -           | 0/6/5/5 |
| 13  | SF4  | l     | 202 | 8    | -       | -           | 0/6/5/5 |
| 13  | SF4  | A     | 707 | 1    | -       | -           | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 13  | SF4  | E     | 502 | 3    | -       | -          | 0/6/5/5 |
| 13  | SF4  | H     | 504 | 12   | -       | -          | 0/6/5/5 |
| 19  | MGD  | H     | 503 | 18   | -       | 8/22/66/66 | 0/6/6/6 |
| 13  | SF4  | a     | 704 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | c     | 202 | 4    | -       | -          | 0/6/5/5 |
| 13  | SF4  | a     | 707 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | K     | 401 | 11   | -       | -          | 0/6/5/5 |
| 13  | SF4  | a     | 703 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | m     | 401 | 11   | -       | -          | 0/6/5/5 |
| 14  | FAD  | A     | 702 | -    | -       | 1/34/50/50 | 0/6/6/6 |
| 13  | SF4  | L     | 201 | 8    | -       | -          | 0/6/5/5 |
| 19  | MGD  | h     | 502 | 18   | -       | 8/22/66/66 | 0/6/6/6 |
| 13  | SF4  | C     | 202 | 4    | -       | -          | 0/6/5/5 |
| 13  | SF4  | E     | 503 | 3    | -       | -          | 0/6/5/5 |
| 13  | SF4  | k     | 405 | 11   | -       | -          | 0/6/5/5 |
| 13  | SF4  | A     | 704 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | A     | 701 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | a     | 701 | 1    | -       | -          | 0/6/5/5 |
| 13  | SF4  | k     | 402 | 11   | -       | -          | 0/6/5/5 |
| 13  | SF4  | m     | 402 | 11   | -       | -          | 0/6/5/5 |

All (132) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 19  | h     | 503 | MGD  | C16-C21 | 12.90  | 1.60        | 1.38     |
| 19  | H     | 503 | MGD  | C16-C21 | 12.84  | 1.60        | 1.38     |
| 19  | H     | 502 | MGD  | C16-C21 | 12.25  | 1.59        | 1.38     |
| 19  | h     | 502 | MGD  | C16-C21 | 12.24  | 1.59        | 1.38     |
| 19  | H     | 503 | MGD  | C14-N15 | 11.02  | 1.58        | 1.46     |
| 19  | h     | 503 | MGD  | C14-N15 | 10.99  | 1.58        | 1.46     |
| 19  | H     | 502 | MGD  | C14-N15 | 10.71  | 1.58        | 1.46     |
| 19  | h     | 502 | MGD  | C14-N15 | 10.67  | 1.58        | 1.46     |
| 19  | h     | 503 | MGD  | C3'-C4' | -10.33 | 1.26        | 1.53     |
| 19  | h     | 502 | MGD  | C3'-C4' | -10.33 | 1.26        | 1.53     |
| 19  | H     | 502 | MGD  | C3'-C4' | -10.32 | 1.26        | 1.53     |
| 19  | H     | 503 | MGD  | C3'-C4' | -10.31 | 1.26        | 1.53     |
| 16  | B     | 302 | 9S8  | S1-FE4  | -9.87  | 2.12        | 2.28     |
| 16  | b     | 302 | 9S8  | S1-FE4  | -9.86  | 2.12        | 2.28     |
| 16  | B     | 301 | 9S8  | S1-FE4  | -9.85  | 2.12        | 2.28     |
| 16  | b     | 301 | 9S8  | S1-FE4  | -9.80  | 2.12        | 2.28     |
| 16  | b     | 301 | 9S8  | S7-FE4  | -9.40  | 2.13        | 2.28     |
| 16  | B     | 301 | 9S8  | S7-FE4  | -9.39  | 2.13        | 2.28     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 302 | 9S8  | S7-FE4  | -9.16 | 2.13        | 2.28     |
| 16  | B     | 302 | 9S8  | S7-FE4  | -9.12 | 2.13        | 2.28     |
| 19  | H     | 502 | MGD  | C2'-C1' | -9.09 | 1.24        | 1.53     |
| 19  | h     | 502 | MGD  | C2'-C1' | -9.09 | 1.24        | 1.53     |
| 19  | h     | 503 | MGD  | C23-C14 | -8.71 | 1.46        | 1.53     |
| 19  | H     | 503 | MGD  | C23-C14 | -8.64 | 1.46        | 1.53     |
| 19  | H     | 502 | MGD  | C23-C14 | -8.60 | 1.46        | 1.53     |
| 19  | h     | 502 | MGD  | C23-C14 | -8.57 | 1.46        | 1.53     |
| 19  | H     | 503 | MGD  | C2'-C1' | -8.56 | 1.26        | 1.53     |
| 19  | h     | 503 | MGD  | C2'-C1' | -8.53 | 1.26        | 1.53     |
| 19  | H     | 503 | MGD  | O11-C23 | -8.50 | 1.31        | 1.43     |
| 19  | h     | 503 | MGD  | O11-C23 | -8.46 | 1.31        | 1.43     |
| 19  | H     | 502 | MGD  | C23-N22 | 7.68  | 1.57        | 1.45     |
| 19  | h     | 502 | MGD  | C23-N22 | 7.67  | 1.57        | 1.45     |
| 19  | h     | 502 | MGD  | O11-C11 | 7.59  | 1.58        | 1.43     |
| 19  | H     | 502 | MGD  | O11-C11 | 7.59  | 1.58        | 1.43     |
| 19  | H     | 502 | MGD  | O11-C23 | -7.50 | 1.32        | 1.43     |
| 19  | h     | 502 | MGD  | O11-C23 | -7.50 | 1.32        | 1.43     |
| 19  | H     | 503 | MGD  | C23-N22 | 7.39  | 1.57        | 1.45     |
| 19  | h     | 503 | MGD  | C23-N22 | 7.36  | 1.57        | 1.45     |
| 19  | h     | 503 | MGD  | O11-C11 | 7.15  | 1.57        | 1.43     |
| 19  | H     | 503 | MGD  | O11-C11 | 7.11  | 1.57        | 1.43     |
| 19  | H     | 503 | MGD  | C19-N18 | 6.77  | 1.54        | 1.37     |
| 19  | h     | 503 | MGD  | C19-N18 | 6.73  | 1.54        | 1.37     |
| 19  | h     | 502 | MGD  | C19-N20 | 6.64  | 1.49        | 1.33     |
| 19  | H     | 502 | MGD  | C19-N20 | 6.63  | 1.49        | 1.33     |
| 19  | H     | 502 | MGD  | C19-N18 | 6.45  | 1.53        | 1.37     |
| 19  | h     | 502 | MGD  | C19-N18 | 6.45  | 1.53        | 1.37     |
| 19  | h     | 503 | MGD  | C4-N3   | 6.30  | 1.48        | 1.34     |
| 19  | H     | 503 | MGD  | C4-N3   | 6.29  | 1.48        | 1.34     |
| 19  | h     | 503 | MGD  | C19-N20 | 6.26  | 1.48        | 1.33     |
| 19  | H     | 503 | MGD  | C19-N20 | 6.22  | 1.48        | 1.33     |
| 19  | H     | 502 | MGD  | C4-N3   | 6.07  | 1.48        | 1.34     |
| 19  | h     | 502 | MGD  | C4-N3   | 6.07  | 1.48        | 1.34     |
| 19  | H     | 503 | MGD  | O4'-C1' | 5.72  | 1.55        | 1.42     |
| 19  | h     | 503 | MGD  | O4'-C1' | 5.68  | 1.55        | 1.42     |
| 19  | h     | 503 | MGD  | C2-N3   | 5.30  | 1.46        | 1.33     |
| 14  | e     | 505 | FAD  | P-O3P   | -5.26 | 1.53        | 1.59     |
| 19  | H     | 503 | MGD  | C2-N3   | 5.25  | 1.45        | 1.33     |
| 14  | E     | 505 | FAD  | P-O3P   | -5.21 | 1.53        | 1.59     |
| 19  | H     | 503 | MGD  | C17-N18 | 4.97  | 1.48        | 1.38     |
| 19  | h     | 503 | MGD  | C17-N18 | 4.95  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | h     | 502 | MGD  | O4'-C1' | 4.87  | 1.53        | 1.42     |
| 19  | H     | 502 | MGD  | O4'-C1' | 4.86  | 1.53        | 1.42     |
| 19  | H     | 502 | MGD  | C17-N18 | 4.81  | 1.47        | 1.38     |
| 19  | h     | 502 | MGD  | C17-N18 | 4.80  | 1.47        | 1.38     |
| 19  | h     | 502 | MGD  | C2-N3   | 4.62  | 1.44        | 1.33     |
| 19  | H     | 502 | MGD  | C2-N3   | 4.61  | 1.44        | 1.33     |
| 19  | h     | 503 | MGD  | C2-N2   | 4.55  | 1.44        | 1.34     |
| 19  | H     | 503 | MGD  | C2-N2   | 4.54  | 1.44        | 1.34     |
| 19  | H     | 503 | MGD  | O4'-C4' | 4.53  | 1.55        | 1.45     |
| 19  | h     | 503 | MGD  | O4'-C4' | 4.52  | 1.55        | 1.45     |
| 19  | H     | 502 | MGD  | C2-N2   | 4.46  | 1.44        | 1.34     |
| 19  | h     | 502 | MGD  | C2-N2   | 4.45  | 1.44        | 1.34     |
| 19  | h     | 502 | MGD  | C21-N20 | 4.44  | 1.43        | 1.36     |
| 19  | H     | 502 | MGD  | C21-N20 | 4.41  | 1.43        | 1.36     |
| 19  | H     | 502 | MGD  | O4'-C4' | 4.34  | 1.54        | 1.45     |
| 19  | h     | 503 | MGD  | C19-N19 | 4.33  | 1.44        | 1.34     |
| 19  | h     | 502 | MGD  | O4'-C4' | 4.32  | 1.54        | 1.45     |
| 19  | H     | 503 | MGD  | C19-N19 | 4.30  | 1.44        | 1.34     |
| 19  | H     | 502 | MGD  | C19-N19 | 4.26  | 1.44        | 1.34     |
| 19  | h     | 502 | MGD  | C19-N19 | 4.25  | 1.44        | 1.34     |
| 19  | H     | 503 | MGD  | C2'-C3' | 4.24  | 1.64        | 1.53     |
| 19  | h     | 503 | MGD  | C2'-C3' | 4.22  | 1.64        | 1.53     |
| 14  | E     | 505 | FAD  | P-O2P   | -4.04 | 1.36        | 1.55     |
| 14  | e     | 505 | FAD  | P-O2P   | -4.04 | 1.36        | 1.55     |
| 19  | h     | 503 | MGD  | PA-O3B  | 4.00  | 1.63        | 1.59     |
| 19  | H     | 502 | MGD  | C21-N22 | 3.95  | 1.39        | 1.35     |
| 19  | h     | 502 | MGD  | C21-N22 | 3.94  | 1.39        | 1.35     |
| 19  | h     | 502 | MGD  | C2'-C3' | 3.93  | 1.64        | 1.53     |
| 19  | H     | 502 | MGD  | C2'-C3' | 3.93  | 1.64        | 1.53     |
| 19  | H     | 503 | MGD  | PA-O3B  | 3.92  | 1.63        | 1.59     |
| 19  | H     | 502 | MGD  | PA-O3B  | 3.75  | 1.63        | 1.59     |
| 19  | h     | 502 | MGD  | PA-O3B  | 3.69  | 1.63        | 1.59     |
| 14  | E     | 505 | FAD  | PA-O5B  | -3.65 | 1.45        | 1.59     |
| 14  | e     | 505 | FAD  | PA-O5B  | -3.64 | 1.45        | 1.59     |
| 19  | h     | 503 | MGD  | PB-O3B  | 3.54  | 1.63        | 1.59     |
| 19  | H     | 503 | MGD  | PB-O3B  | 3.54  | 1.63        | 1.59     |
| 19  | h     | 502 | MGD  | PB-O3B  | 3.50  | 1.63        | 1.59     |
| 19  | H     | 502 | MGD  | PB-O3B  | 3.48  | 1.63        | 1.59     |
| 19  | h     | 502 | MGD  | C5-N7   | -3.44 | 1.32        | 1.39     |
| 19  | H     | 502 | MGD  | C5-N7   | -3.41 | 1.32        | 1.39     |
| 19  | H     | 503 | MGD  | C21-N20 | 3.36  | 1.41        | 1.36     |
| 19  | h     | 503 | MGD  | C21-N20 | 3.34  | 1.41        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 702 | FAD  | P-O2P   | -3.23 | 1.40        | 1.55     |
| 14  | a     | 702 | FAD  | P-O2P   | -3.22 | 1.40        | 1.55     |
| 19  | h     | 502 | MGD  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 19  | H     | 502 | MGD  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 19  | H     | 503 | MGD  | C5-N7   | -3.13 | 1.32        | 1.39     |
| 19  | h     | 503 | MGD  | C5-N7   | -3.09 | 1.32        | 1.39     |
| 19  | h     | 502 | MGD  | C4-N9   | -3.04 | 1.30        | 1.38     |
| 19  | H     | 502 | MGD  | C4-N9   | -3.01 | 1.30        | 1.38     |
| 19  | h     | 502 | MGD  | O17-C17 | -2.96 | 1.17        | 1.23     |
| 19  | H     | 502 | MGD  | O17-C17 | -2.96 | 1.18        | 1.23     |
| 14  | A     | 702 | FAD  | P-O3P   | -2.79 | 1.56        | 1.59     |
| 14  | a     | 702 | FAD  | P-O3P   | -2.79 | 1.56        | 1.59     |
| 19  | h     | 503 | MGD  | O17-C17 | -2.76 | 1.18        | 1.23     |
| 19  | h     | 503 | MGD  | O6-C6   | -2.76 | 1.18        | 1.23     |
| 19  | H     | 503 | MGD  | O6-C6   | -2.75 | 1.18        | 1.23     |
| 19  | H     | 503 | MGD  | O17-C17 | -2.74 | 1.18        | 1.23     |
| 19  | H     | 503 | MGD  | C21-N22 | 2.68  | 1.38        | 1.35     |
| 19  | h     | 503 | MGD  | C21-N22 | 2.67  | 1.38        | 1.35     |
| 19  | H     | 503 | MGD  | C16-C17 | 2.39  | 1.49        | 1.41     |
| 19  | h     | 503 | MGD  | C16-C17 | 2.39  | 1.49        | 1.41     |
| 19  | H     | 503 | MGD  | C2-N1   | 2.35  | 1.43        | 1.37     |
| 19  | H     | 503 | MGD  | C5-C6   | 2.34  | 1.53        | 1.44     |
| 19  | h     | 503 | MGD  | C5-C6   | 2.33  | 1.53        | 1.44     |
| 19  | h     | 503 | MGD  | C2-N1   | 2.32  | 1.43        | 1.37     |
| 19  | H     | 503 | MGD  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 14  | a     | 702 | FAD  | C4-N3   | -2.19 | 1.34        | 1.38     |
| 19  | h     | 503 | MGD  | C4-N9   | -2.18 | 1.32        | 1.38     |
| 14  | A     | 702 | FAD  | C4-N3   | -2.17 | 1.34        | 1.38     |
| 19  | H     | 502 | MGD  | C10-C11 | 2.15  | 1.54        | 1.51     |
| 19  | h     | 502 | MGD  | C10-C11 | 2.15  | 1.54        | 1.51     |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | h     | 502 | MGD  | O11-C23-N22 | -6.39 | 102.81      | 108.61   |
| 19  | H     | 502 | MGD  | O11-C23-N22 | -6.38 | 102.81      | 108.61   |
| 19  | H     | 503 | MGD  | C23-C14-N15 | 5.79  | 113.56      | 107.87   |
| 19  | h     | 503 | MGD  | C23-C14-N15 | 5.79  | 113.55      | 107.87   |
| 19  | H     | 503 | MGD  | C5-C4-N3    | -5.38 | 119.82      | 128.39   |
| 19  | h     | 503 | MGD  | C5-C4-N3    | -5.38 | 119.82      | 128.39   |
| 19  | h     | 502 | MGD  | C23-C14-N15 | 4.71  | 112.49      | 107.87   |
| 19  | H     | 502 | MGD  | C23-C14-N15 | 4.68  | 112.46      | 107.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | H     | 503 | MGD  | C2-N3-C4    | 4.63  | 120.28      | 112.30   |
| 19  | h     | 503 | MGD  | C2-N3-C4    | 4.60  | 120.22      | 112.30   |
| 19  | h     | 502 | MGD  | C2-N3-C4    | 4.11  | 119.38      | 112.30   |
| 19  | H     | 502 | MGD  | C2-N3-C4    | 4.09  | 119.34      | 112.30   |
| 19  | h     | 502 | MGD  | C19-N20-C21 | 4.03  | 120.47      | 113.36   |
| 19  | h     | 502 | MGD  | C5-C4-N3    | -4.02 | 121.99      | 128.39   |
| 19  | H     | 502 | MGD  | C19-N20-C21 | 4.02  | 120.45      | 113.36   |
| 19  | H     | 502 | MGD  | C5-C4-N3    | -4.02 | 122.00      | 128.39   |
| 19  | H     | 503 | MGD  | C19-N20-C21 | 3.83  | 120.11      | 113.36   |
| 19  | h     | 503 | MGD  | C19-N20-C21 | 3.81  | 120.09      | 113.36   |
| 19  | H     | 502 | MGD  | N9-C8-N7    | -3.42 | 107.06      | 113.40   |
| 19  | h     | 502 | MGD  | N9-C8-N7    | -3.42 | 107.07      | 113.40   |
| 19  | H     | 503 | MGD  | C2-N1-C6    | -3.33 | 119.08      | 125.11   |
| 19  | h     | 503 | MGD  | C2-N1-C6    | -3.32 | 119.09      | 125.11   |
| 19  | h     | 503 | MGD  | N19-C19-N18 | 3.25  | 123.61      | 116.76   |
| 19  | H     | 503 | MGD  | N19-C19-N18 | 3.23  | 123.58      | 116.76   |
| 19  | H     | 503 | MGD  | N9-C4-N3    | 3.23  | 132.41      | 125.95   |
| 19  | H     | 502 | MGD  | O17-C17-C16 | -3.22 | 119.50      | 127.26   |
| 19  | h     | 502 | MGD  | O17-C17-C16 | -3.21 | 119.51      | 127.26   |
| 19  | h     | 503 | MGD  | N9-C4-N3    | 3.20  | 132.35      | 125.95   |
| 19  | h     | 503 | MGD  | N9-C8-N7    | -3.20 | 107.47      | 113.40   |
| 19  | H     | 503 | MGD  | N9-C8-N7    | -3.19 | 107.49      | 113.40   |
| 19  | H     | 502 | MGD  | C4'-O4'-C1' | -3.02 | 102.79      | 109.47   |
| 19  | h     | 502 | MGD  | C4'-O4'-C1' | -3.01 | 102.81      | 109.47   |
| 19  | H     | 502 | MGD  | C19-N18-C17 | -2.91 | 119.84      | 125.11   |
| 19  | H     | 502 | MGD  | C16-C17-N18 | 2.89  | 120.08      | 112.13   |
| 19  | h     | 502 | MGD  | C16-C17-N18 | 2.89  | 120.07      | 112.13   |
| 19  | h     | 502 | MGD  | C19-N18-C17 | -2.89 | 119.87      | 125.11   |
| 19  | H     | 503 | MGD  | C5-C6-N1    | 2.84  | 120.49      | 113.25   |
| 19  | h     | 503 | MGD  | C5-C6-N1    | 2.82  | 120.44      | 113.25   |
| 19  | H     | 502 | MGD  | C1'-N9-C4   | -2.75 | 118.37      | 126.49   |
| 19  | h     | 502 | MGD  | C1'-N9-C4   | -2.74 | 118.40      | 126.49   |
| 19  | h     | 503 | MGD  | C16-C17-N18 | 2.60  | 119.27      | 112.13   |
| 19  | H     | 503 | MGD  | C16-C17-N18 | 2.59  | 119.24      | 112.13   |
| 19  | h     | 502 | MGD  | N1-C2-N3    | -2.52 | 118.71      | 123.32   |
| 19  | H     | 503 | MGD  | C19-N18-C17 | -2.50 | 120.58      | 125.11   |
| 19  | H     | 502 | MGD  | N1-C2-N3    | -2.49 | 118.76      | 123.32   |
| 19  | h     | 503 | MGD  | C19-N18-C17 | -2.49 | 120.59      | 125.11   |
| 19  | H     | 502 | MGD  | C5-C6-N1    | 2.46  | 119.50      | 113.25   |
| 19  | H     | 502 | MGD  | N9-C4-N3    | 2.45  | 130.86      | 125.95   |
| 19  | h     | 502 | MGD  | N9-C4-N3    | 2.45  | 130.85      | 125.95   |
| 19  | h     | 502 | MGD  | C5-C6-N1    | 2.45  | 119.48      | 113.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | h     | 503 | MGD  | O17-C17-C16 | -2.44 | 121.37      | 127.26   |
| 19  | H     | 503 | MGD  | O17-C17-C16 | -2.41 | 121.44      | 127.26   |
| 19  | H     | 503 | MGD  | O6-C6-C5    | -2.29 | 120.50      | 126.53   |
| 19  | h     | 503 | MGD  | O6-C6-C5    | -2.28 | 120.50      | 126.53   |
| 19  | h     | 502 | MGD  | O6-C6-C5    | -2.20 | 120.72      | 126.53   |
| 19  | h     | 503 | MGD  | C8-N7-C5    | 2.20  | 108.18      | 104.26   |
| 19  | H     | 502 | MGD  | O6-C6-C5    | -2.20 | 120.73      | 126.53   |
| 19  | H     | 503 | MGD  | C8-N7-C5    | 2.19  | 108.16      | 104.26   |
| 19  | h     | 503 | MGD  | O4'-C1'-C2' | -2.17 | 101.96      | 106.62   |
| 19  | H     | 503 | MGD  | O4'-C1'-C2' | -2.14 | 102.03      | 106.62   |
| 19  | h     | 503 | MGD  | C17-C16-N15 | 2.12  | 122.05      | 116.27   |
| 19  | H     | 503 | MGD  | C17-C16-N15 | 2.09  | 121.97      | 116.27   |
| 19  | H     | 503 | MGD  | C4'-O4'-C1' | -2.01 | 105.02      | 109.47   |

There are no chirality outliers.

All (60) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | E     | 505 | FAD  | C5B-O5B-PA-O1A  |
| 14  | E     | 505 | FAD  | C5B-O5B-PA-O3P  |
| 14  | E     | 505 | FAD  | C1'-C2'-C3'-O3' |
| 14  | E     | 505 | FAD  | C1'-C2'-C3'-C4' |
| 14  | E     | 505 | FAD  | O2'-C2'-C3'-O3' |
| 14  | E     | 505 | FAD  | O2'-C2'-C3'-C4' |
| 14  | E     | 505 | FAD  | C5'-O5'-P-O2P   |
| 14  | E     | 505 | FAD  | C5'-O5'-P-O3P   |
| 14  | e     | 505 | FAD  | C5B-O5B-PA-O1A  |
| 14  | e     | 505 | FAD  | C5B-O5B-PA-O3P  |
| 14  | e     | 505 | FAD  | C1'-C2'-C3'-O3' |
| 14  | e     | 505 | FAD  | C1'-C2'-C3'-C4' |
| 14  | e     | 505 | FAD  | O2'-C2'-C3'-O3' |
| 14  | e     | 505 | FAD  | O2'-C2'-C3'-C4' |
| 14  | e     | 505 | FAD  | C5'-O5'-P-O2P   |
| 14  | e     | 505 | FAD  | C5'-O5'-P-O3P   |
| 19  | H     | 502 | MGD  | C5'-O5'-PB-O3B  |
| 19  | H     | 502 | MGD  | PB-O3B-PA-O3A   |
| 19  | H     | 502 | MGD  | C10-O3A-PA-O3B  |
| 19  | H     | 502 | MGD  | C10-O3A-PA-O1A  |
| 19  | H     | 502 | MGD  | C10-O3A-PA-O2A  |
| 19  | H     | 502 | MGD  | O3A-C10-C11-O11 |
| 19  | H     | 502 | MGD  | O3A-C10-C11-C12 |
| 19  | H     | 503 | MGD  | C5'-O5'-PB-O2B  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | H     | 503 | MGD  | C5'-O5'-PB-O3B  |
| 19  | h     | 502 | MGD  | C5'-O5'-PB-O3B  |
| 19  | h     | 502 | MGD  | PB-O3B-PA-O3A   |
| 19  | h     | 502 | MGD  | C10-O3A-PA-O3B  |
| 19  | h     | 502 | MGD  | C10-O3A-PA-O1A  |
| 19  | h     | 502 | MGD  | C10-O3A-PA-O2A  |
| 19  | h     | 502 | MGD  | O3A-C10-C11-O11 |
| 19  | h     | 502 | MGD  | O3A-C10-C11-C12 |
| 19  | h     | 503 | MGD  | C5'-O5'-PB-O2B  |
| 19  | h     | 503 | MGD  | C5'-O5'-PB-O3B  |
| 19  | H     | 503 | MGD  | C3'-C4'-C5'-O5' |
| 19  | h     | 503 | MGD  | C3'-C4'-C5'-O5' |
| 19  | H     | 503 | MGD  | O4'-C4'-C5'-O5' |
| 19  | h     | 503 | MGD  | O4'-C4'-C5'-O5' |
| 14  | E     | 505 | FAD  | C5B-O5B-PA-O2A  |
| 14  | e     | 505 | FAD  | C5B-O5B-PA-O2A  |
| 19  | H     | 503 | MGD  | C5'-O5'-PB-O1B  |
| 19  | H     | 503 | MGD  | C10-O3A-PA-O2A  |
| 19  | h     | 503 | MGD  | C5'-O5'-PB-O1B  |
| 19  | h     | 503 | MGD  | C10-O3A-PA-O2A  |
| 19  | H     | 503 | MGD  | PB-O3B-PA-O2A   |
| 19  | h     | 503 | MGD  | PB-O3B-PA-O2A   |
| 14  | E     | 505 | FAD  | C4'-C5'-O5'-P   |
| 14  | e     | 505 | FAD  | C4'-C5'-O5'-P   |
| 19  | H     | 503 | MGD  | PB-O3B-PA-O1A   |
| 19  | h     | 503 | MGD  | PB-O3B-PA-O1A   |
| 19  | H     | 502 | MGD  | O4'-C4'-C5'-O5' |
| 19  | h     | 502 | MGD  | O4'-C4'-C5'-O5' |
| 14  | E     | 505 | FAD  | C2B-C1B-N9A-C8A |
| 14  | e     | 505 | FAD  | C2B-C1B-N9A-C8A |
| 14  | E     | 505 | FAD  | N10-C1'-C2'-O2' |
| 14  | e     | 505 | FAD  | N10-C1'-C2'-O2' |
| 14  | E     | 505 | FAD  | P-O3P-PA-O2A    |
| 14  | e     | 505 | FAD  | P-O3P-PA-O2A    |
| 14  | A     | 702 | FAD  | O4B-C4B-C5B-O5B |
| 14  | a     | 702 | FAD  | O4B-C4B-C5B-O5B |

There are no ring outliers.

13 monomers are involved in 27 short contacts:

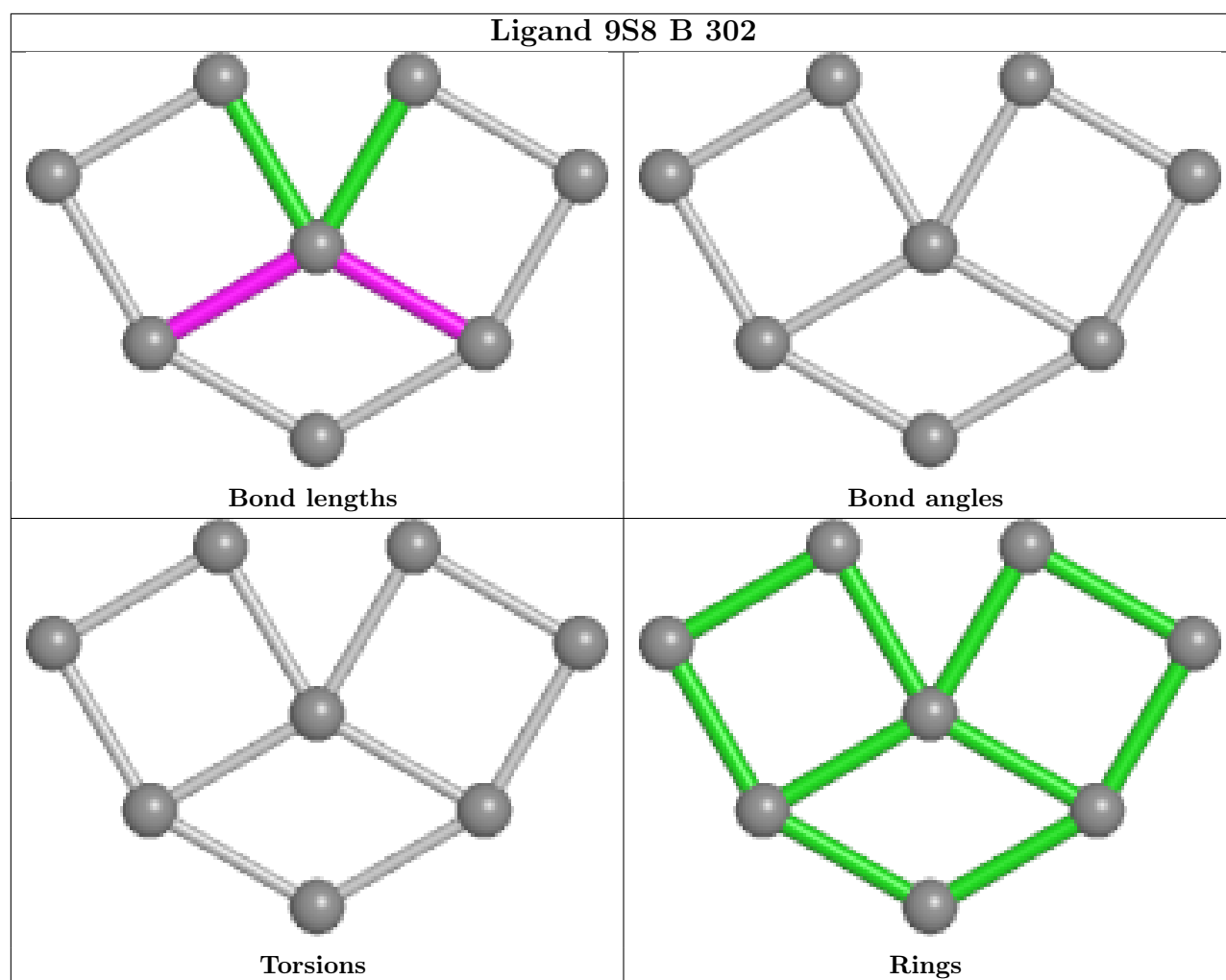
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | C     | 201 | SF4  | 1       | 0            |

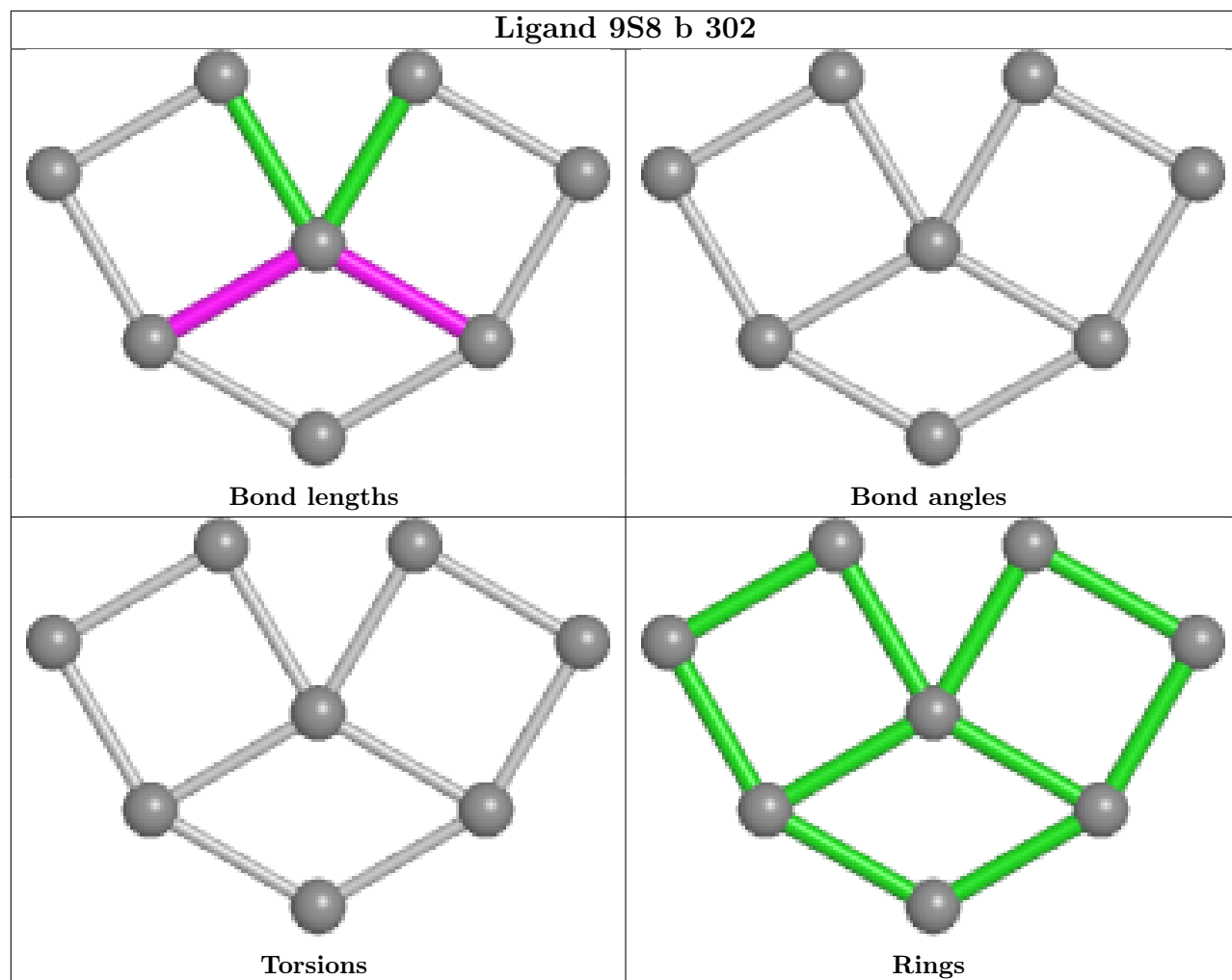
*Continued on next page...*

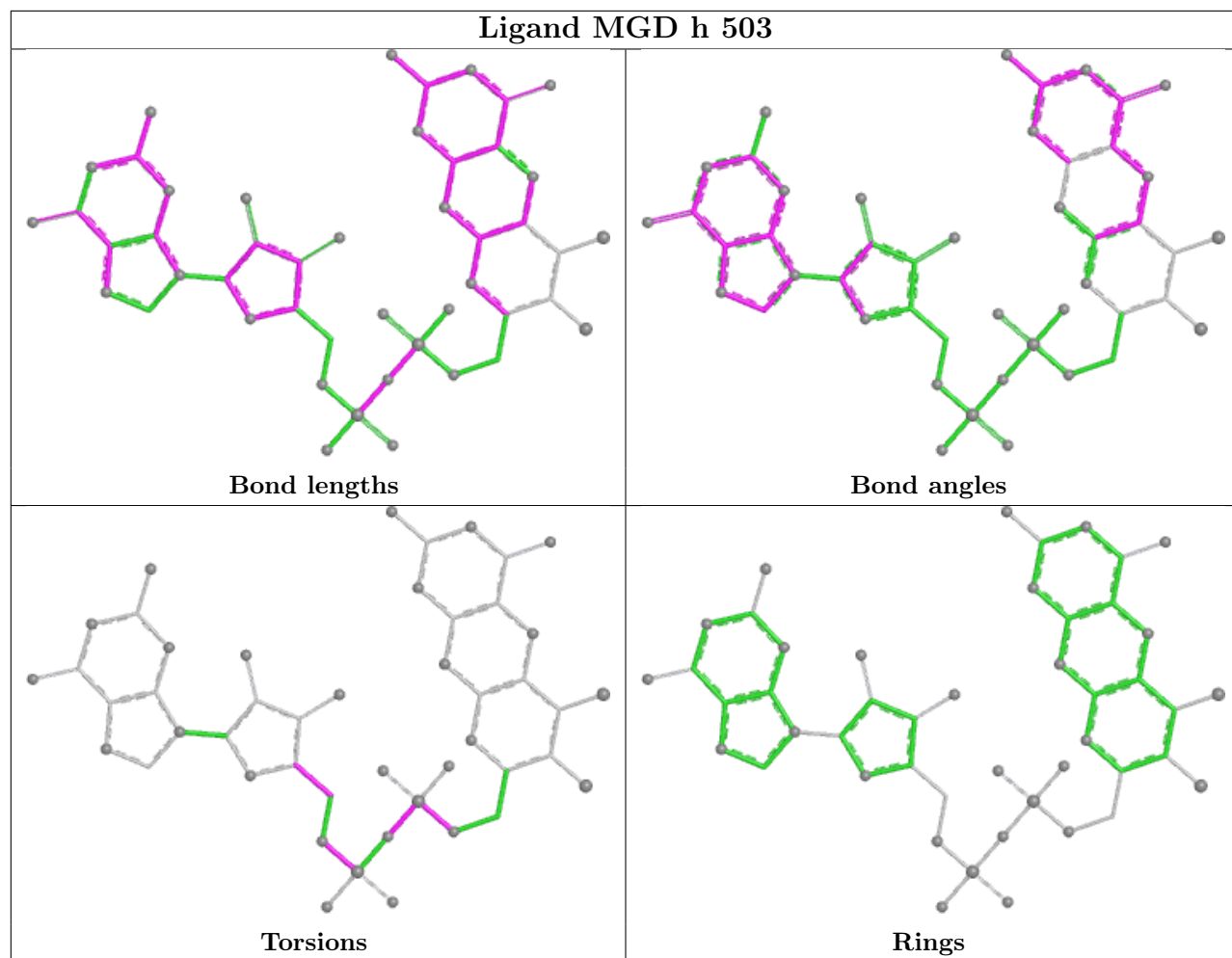
*Continued from previous page...*

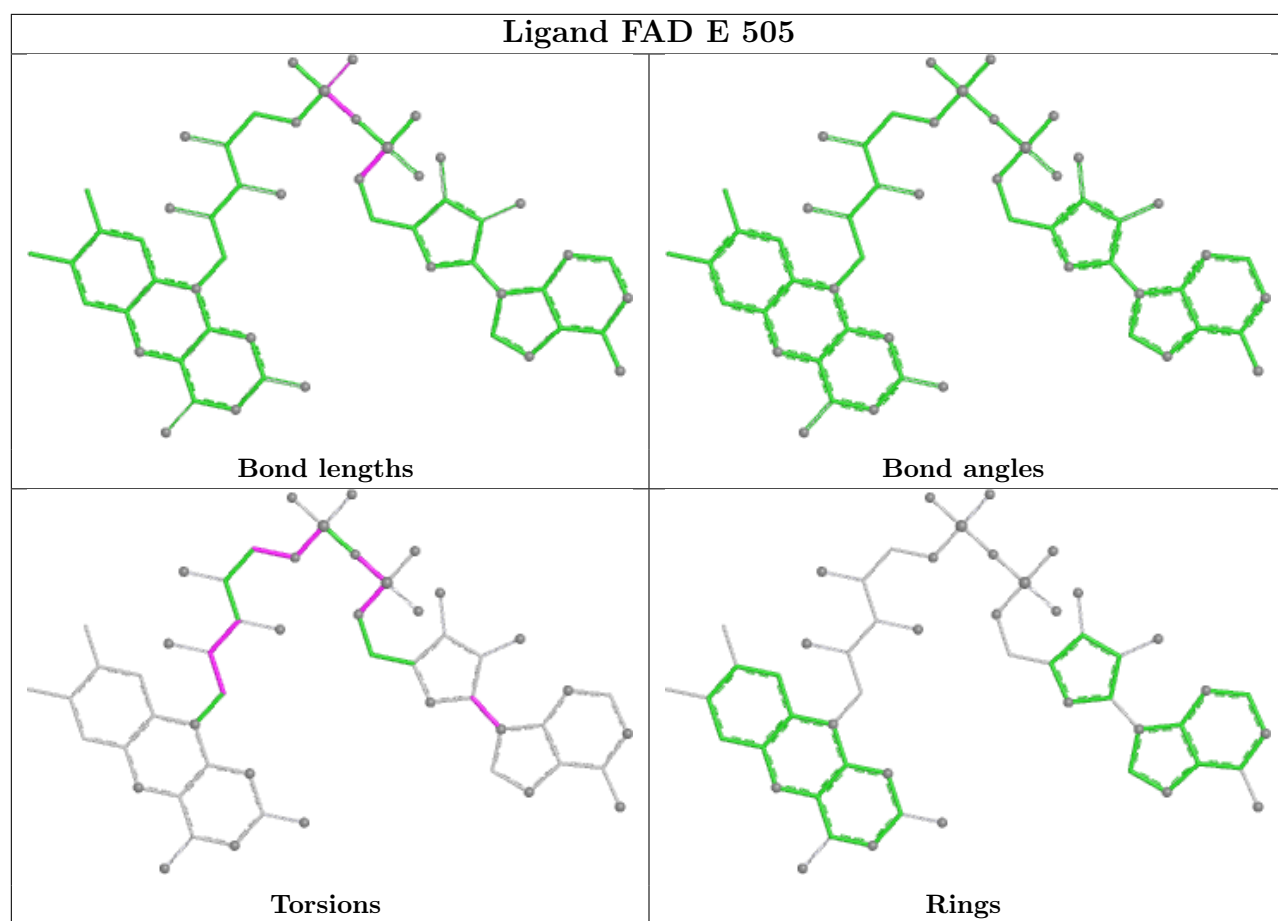
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | B     | 302 | 9S8  | 1       | 0            |
| 16  | b     | 302 | 9S8  | 1       | 0            |
| 19  | h     | 503 | MGD  | 2       | 0            |
| 14  | E     | 505 | FAD  | 1       | 0            |
| 13  | A     | 703 | SF4  | 2       | 0            |
| 19  | H     | 502 | MGD  | 6       | 0            |
| 13  | c     | 201 | SF4  | 1       | 0            |
| 13  | K     | 405 | SF4  | 1       | 0            |
| 19  | H     | 503 | MGD  | 2       | 0            |
| 13  | a     | 703 | SF4  | 2       | 0            |
| 19  | h     | 502 | MGD  | 6       | 0            |
| 13  | k     | 405 | SF4  | 1       | 0            |

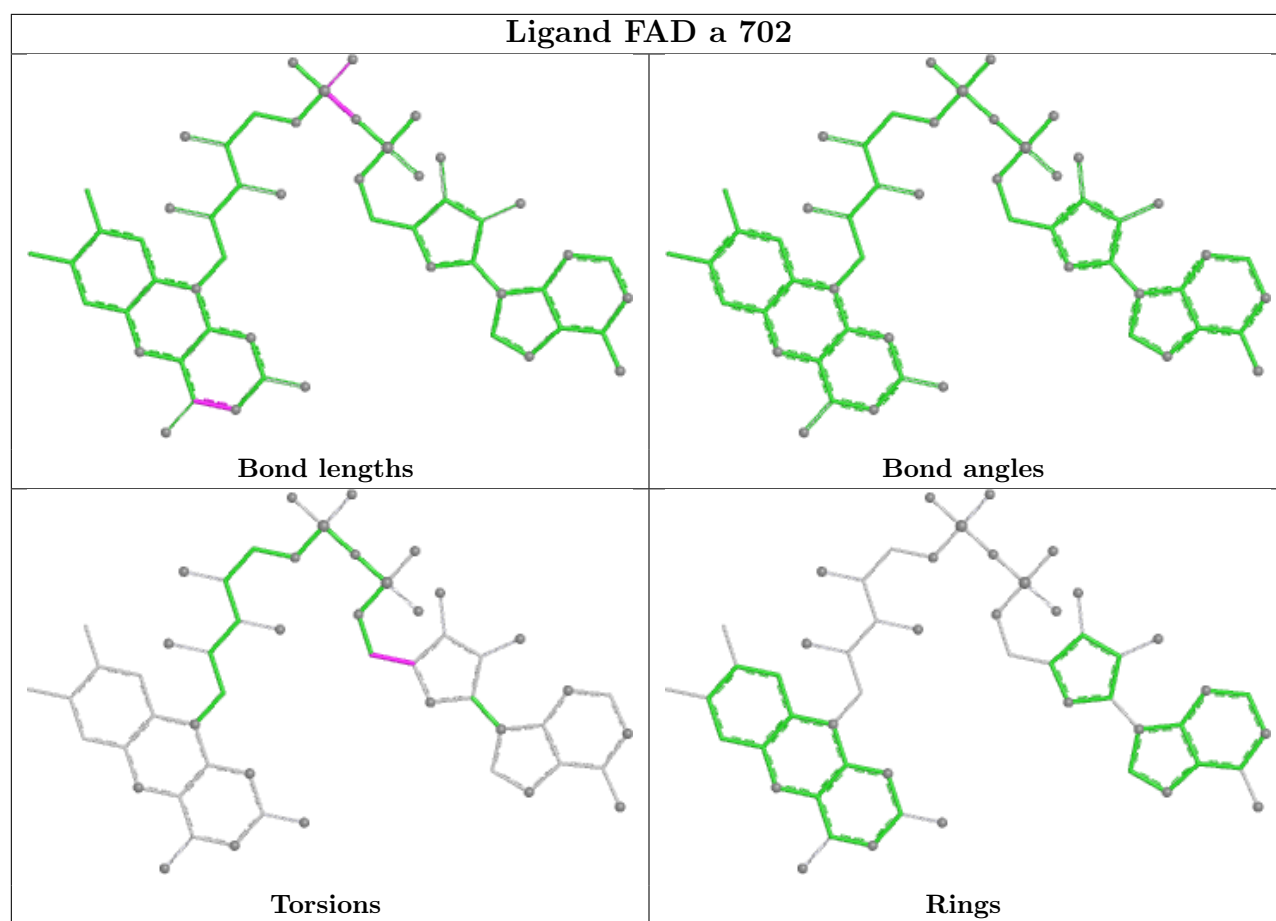
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

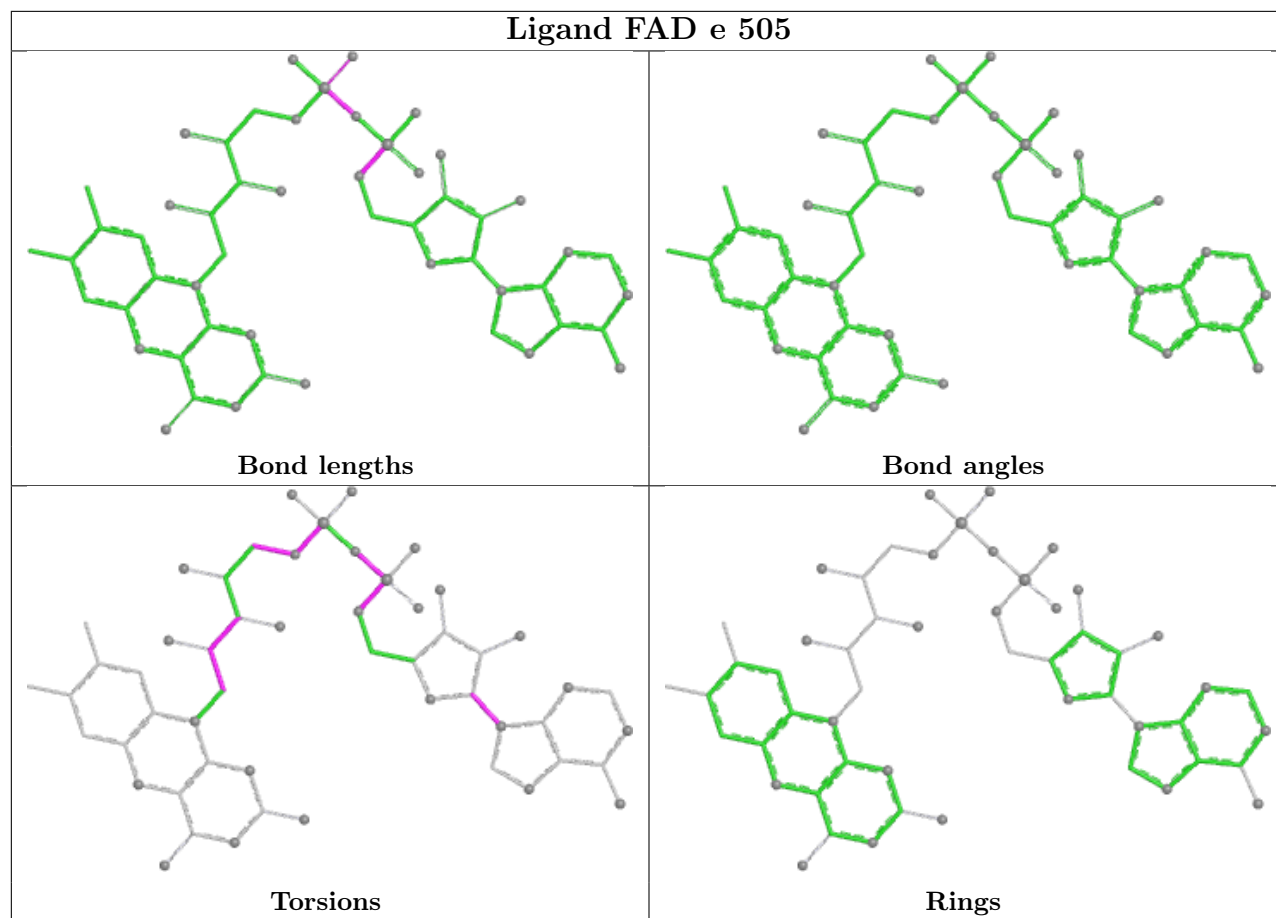


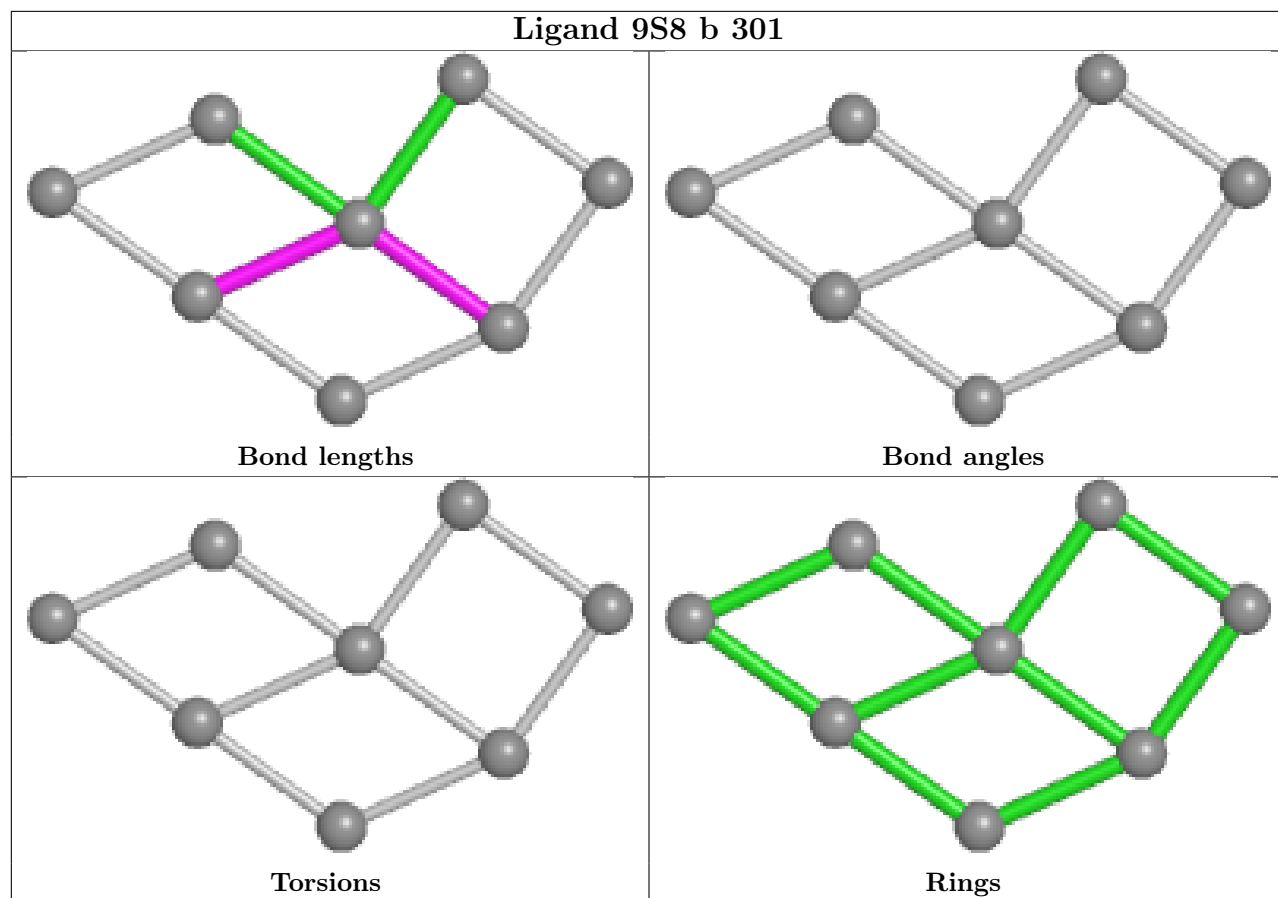


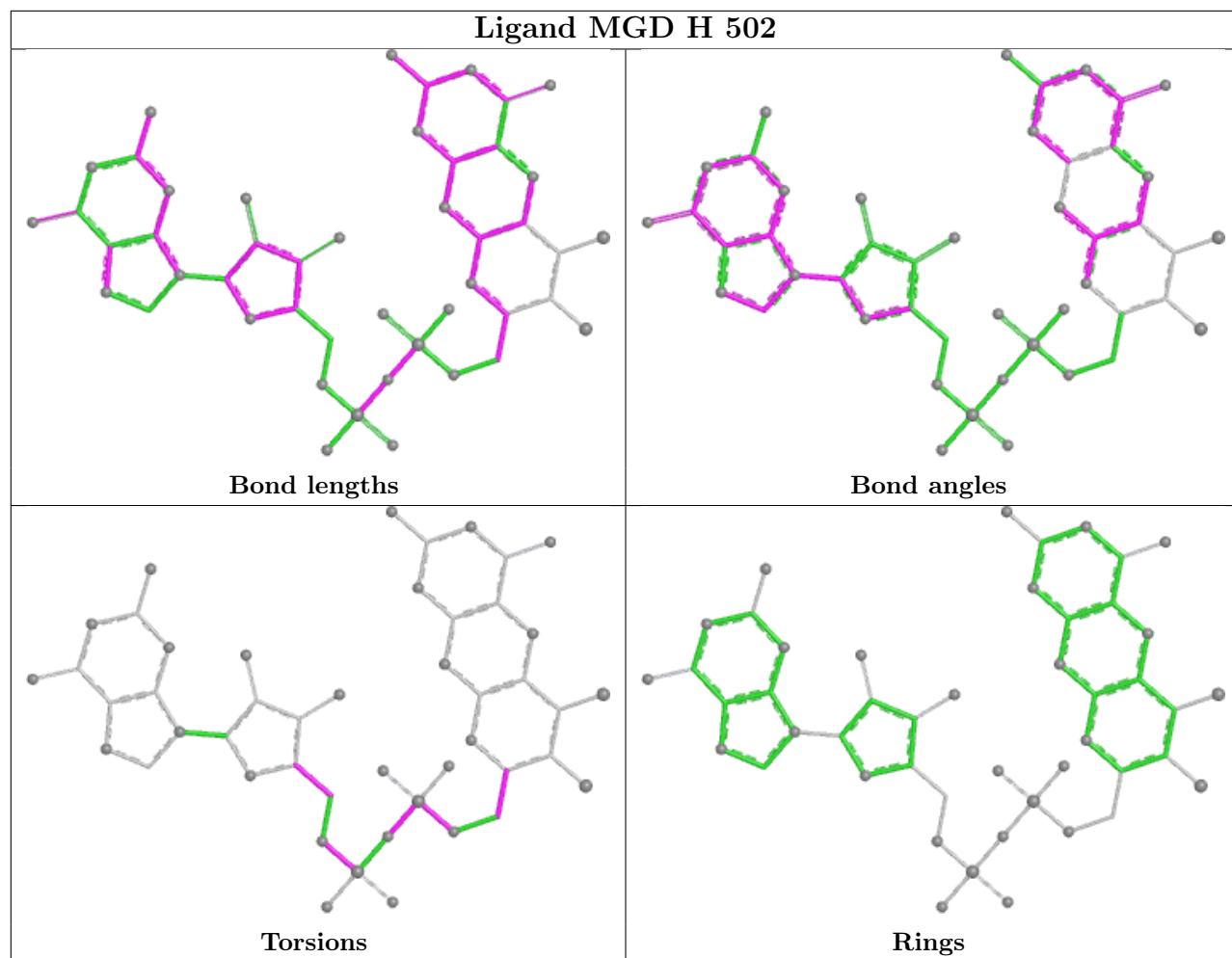


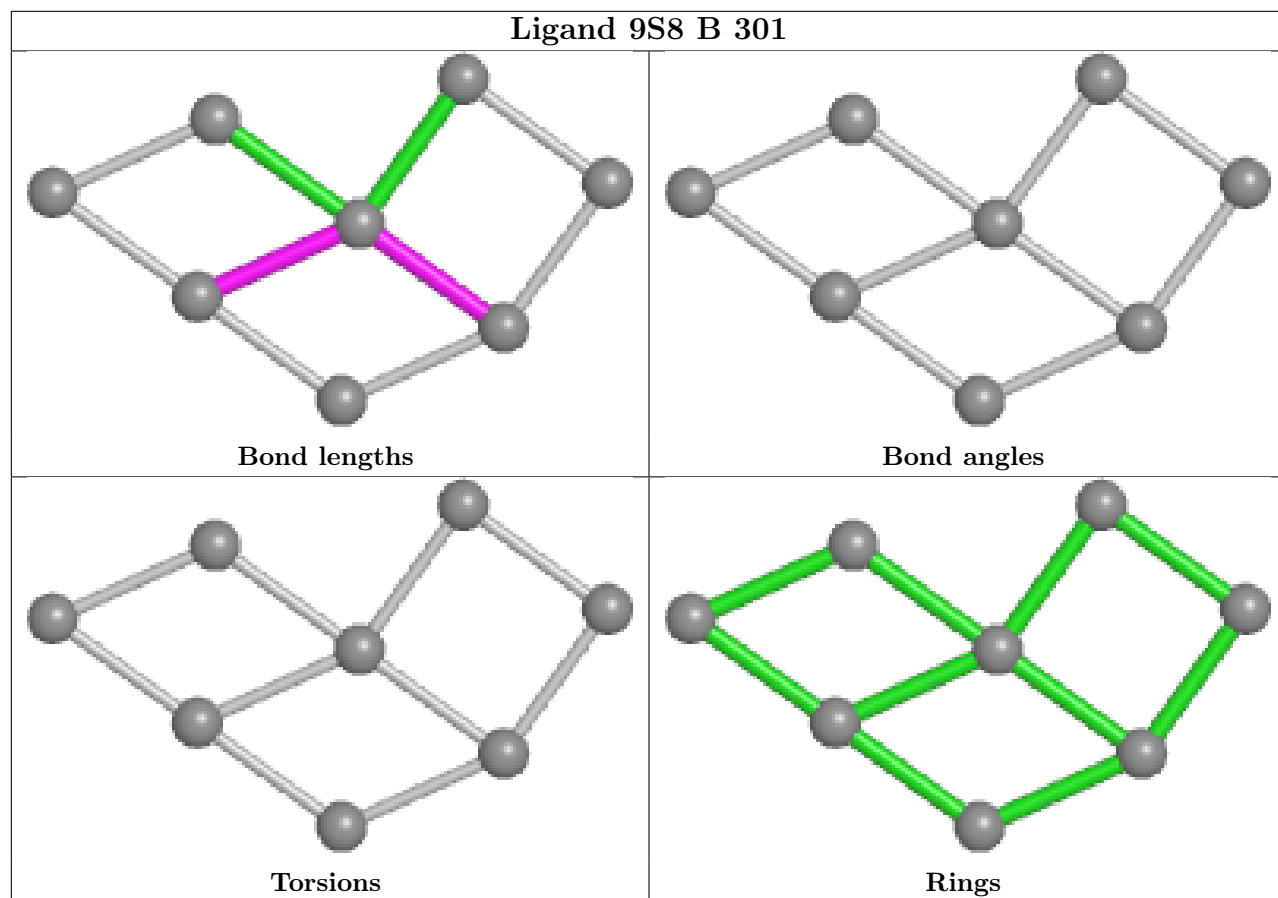


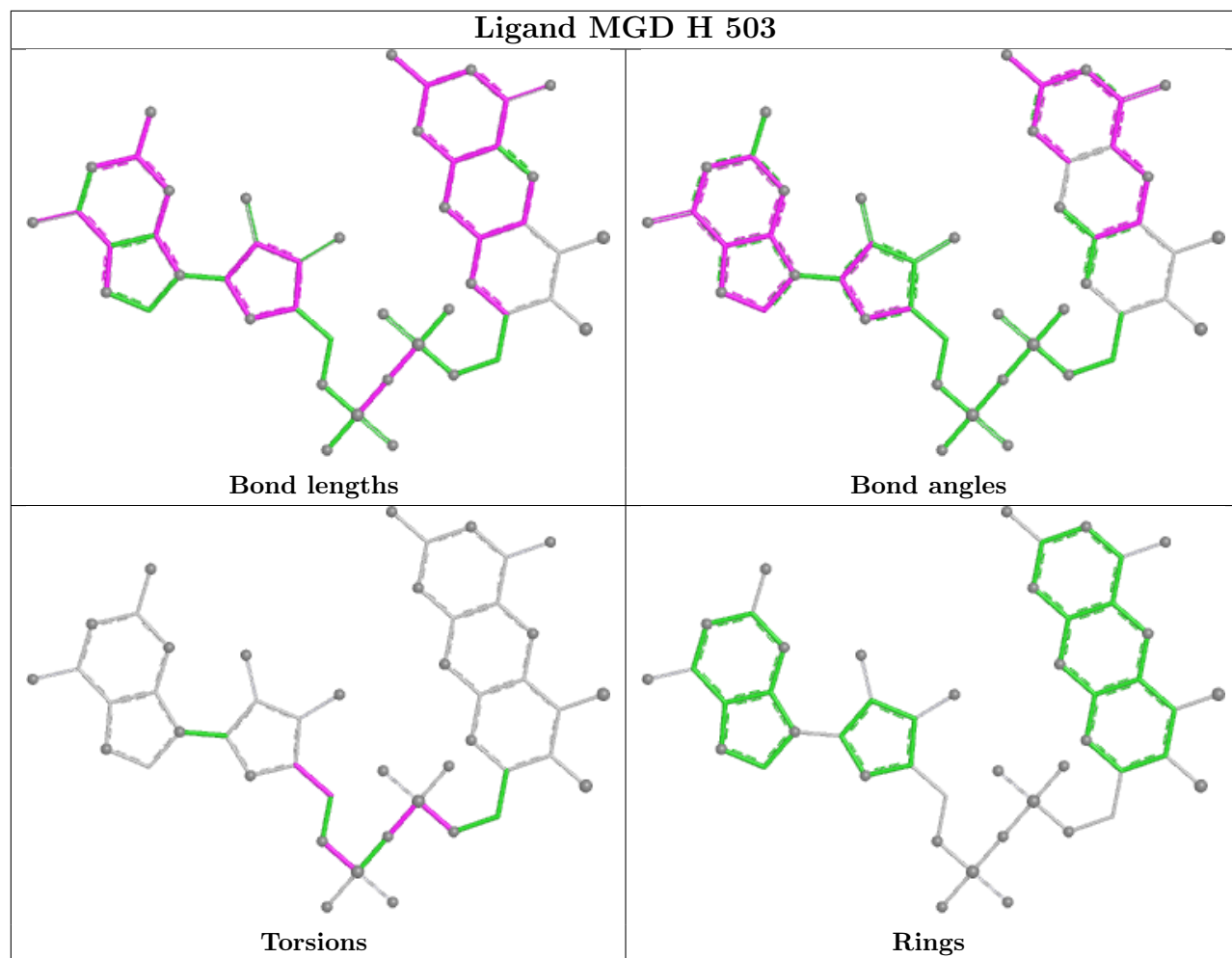


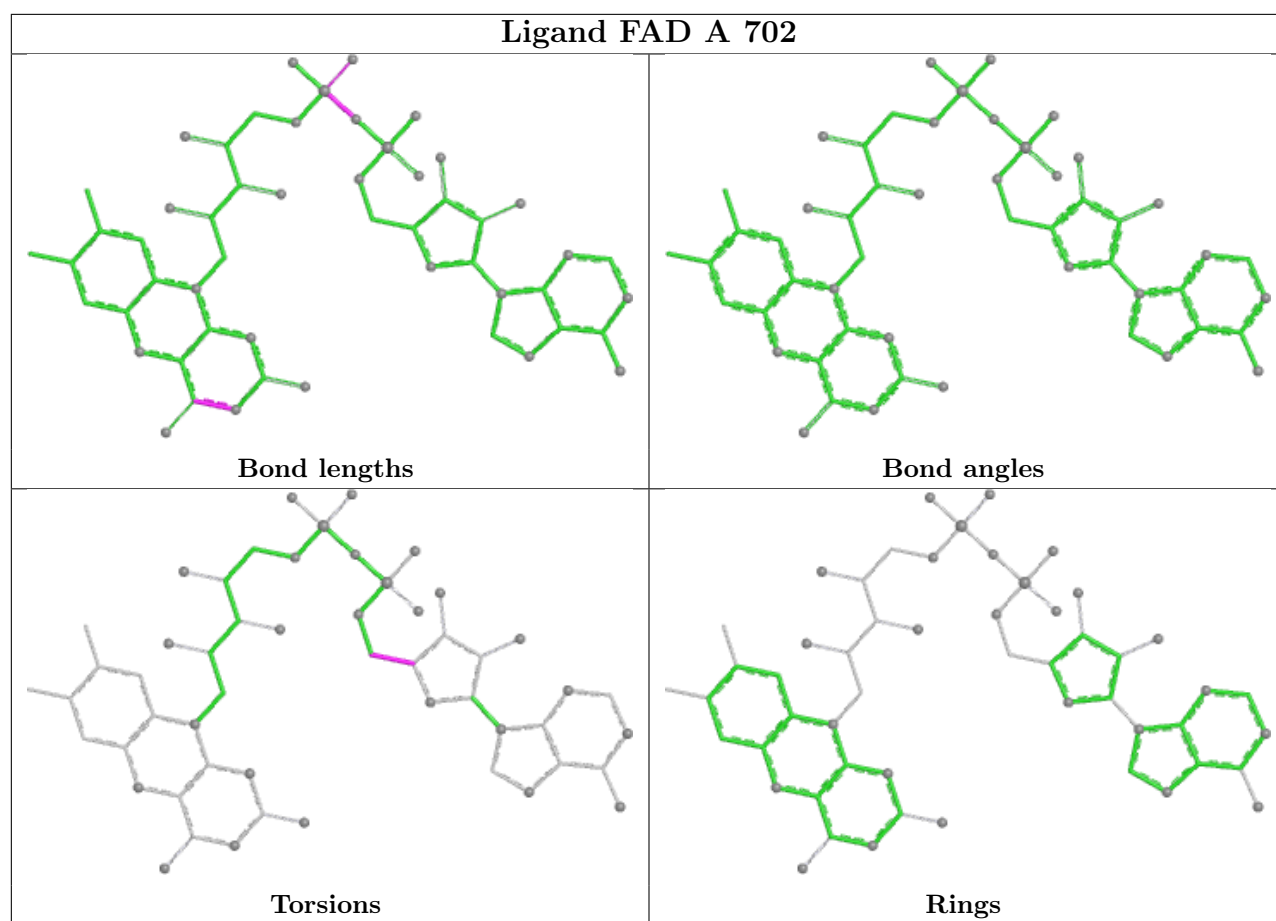


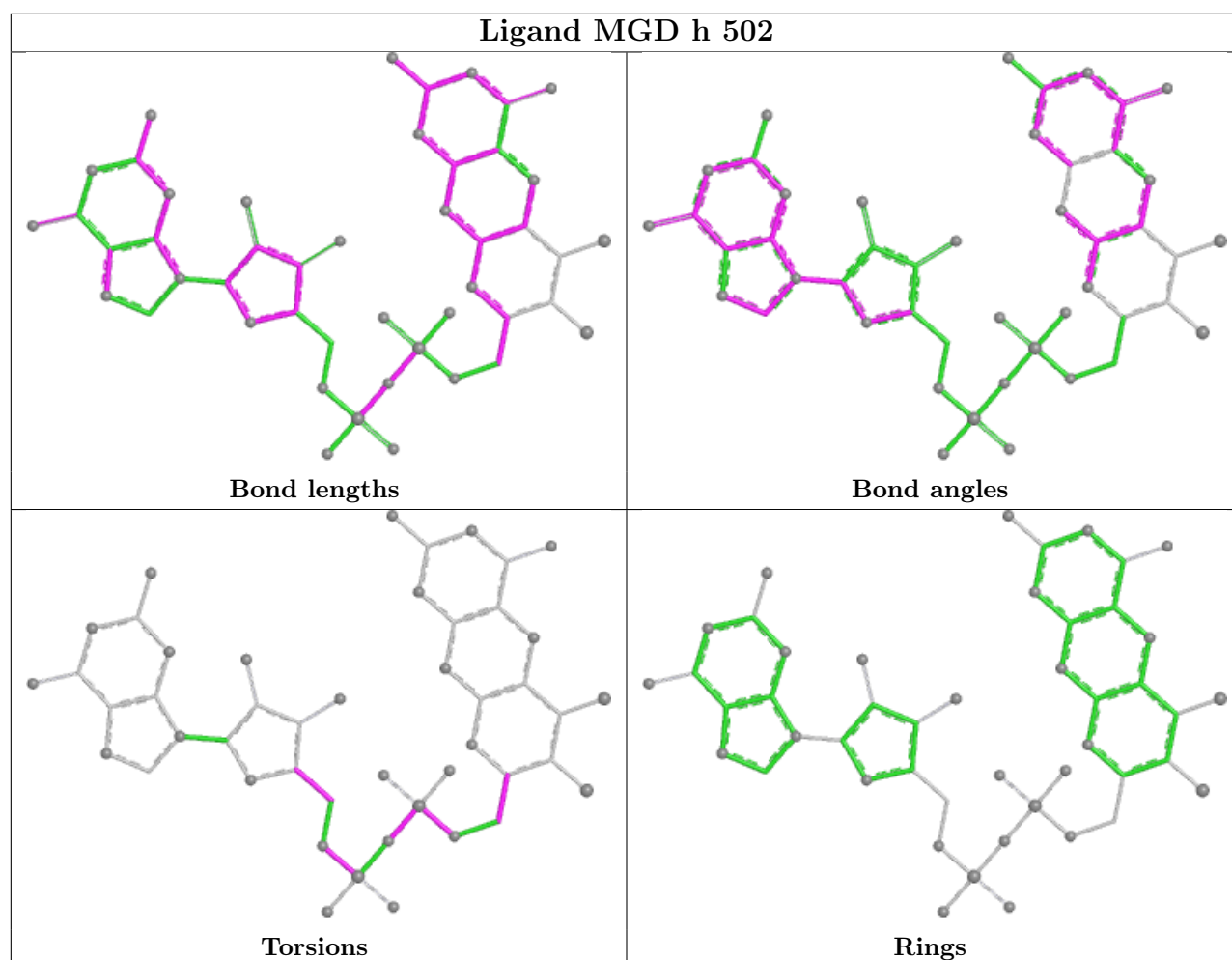












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

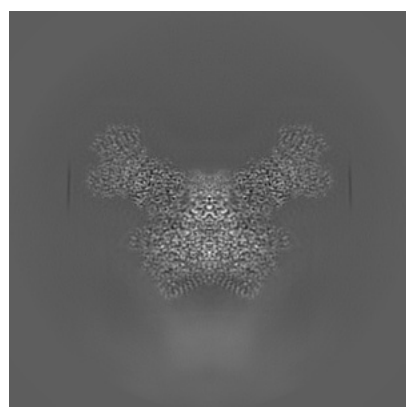
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12209. These allow visual inspection of the internal detail of the map and identification of artifacts.

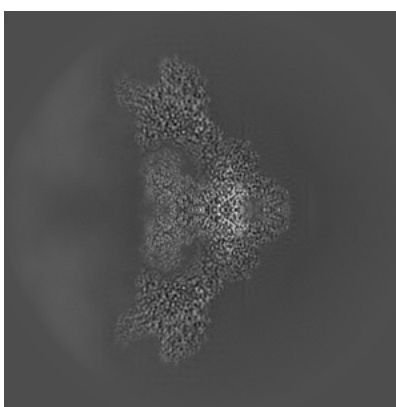
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

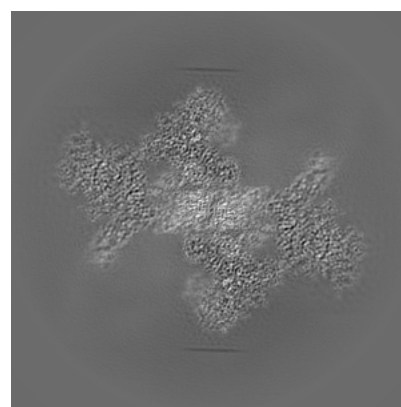
#### 6.1.1 Primary map



X



Y

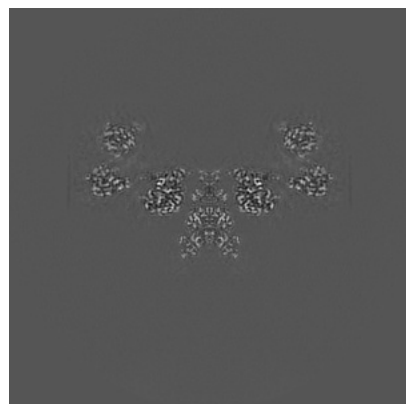


Z

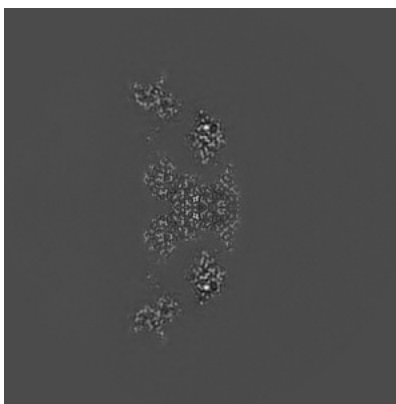
The images above show the map projected in three orthogonal directions.

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

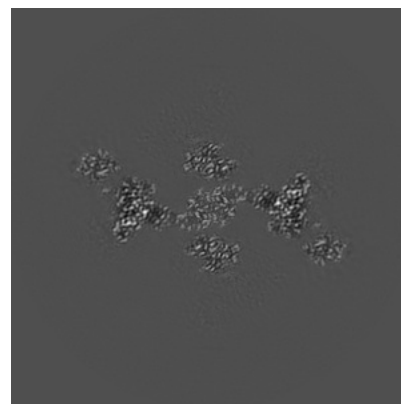
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

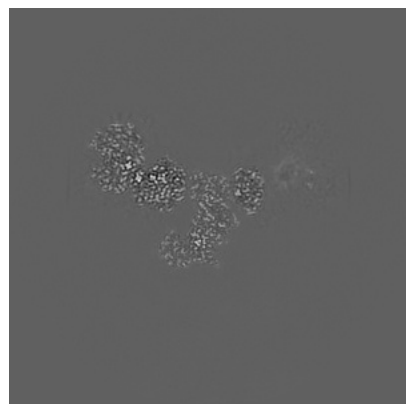


Z Index: 216

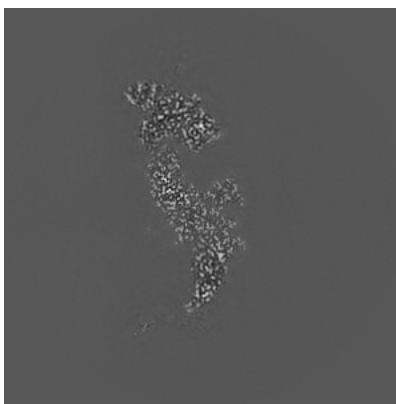
The images above show central slices of the map in three orthogonal directions.

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

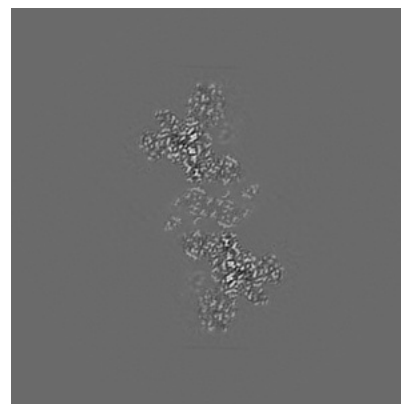
### 6.3.1 Primary map



X Index: 235



Y Index: 202

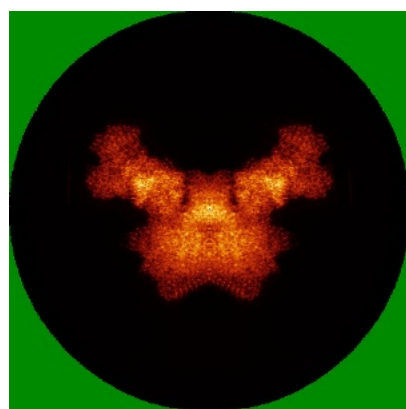


Z Index: 248

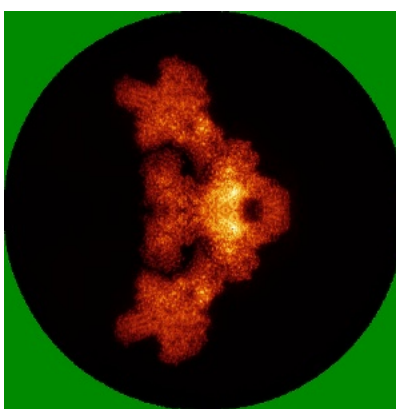
The images above show the largest variance slices of the map in three orthogonal directions.

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

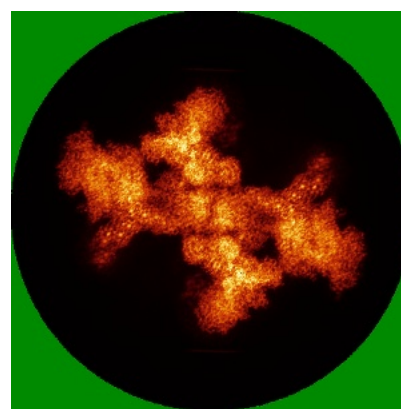
### 6.4.1 Primary map



X



Y

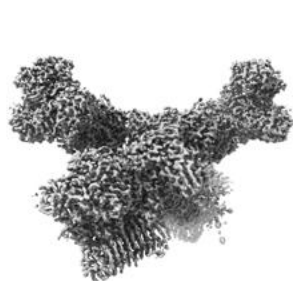


Z

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](#)

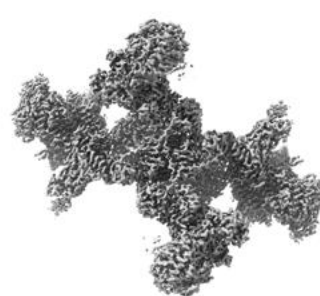
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

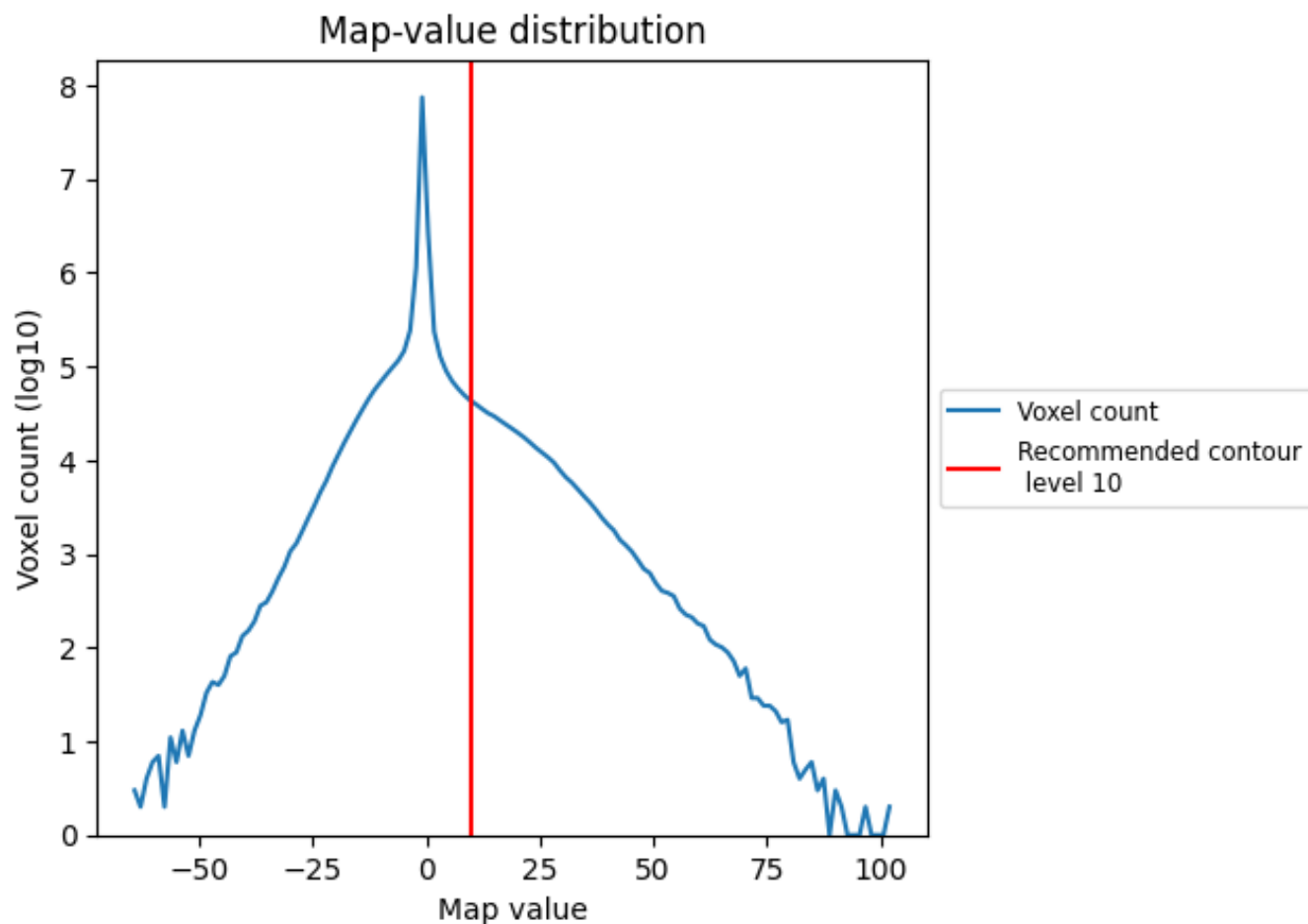
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

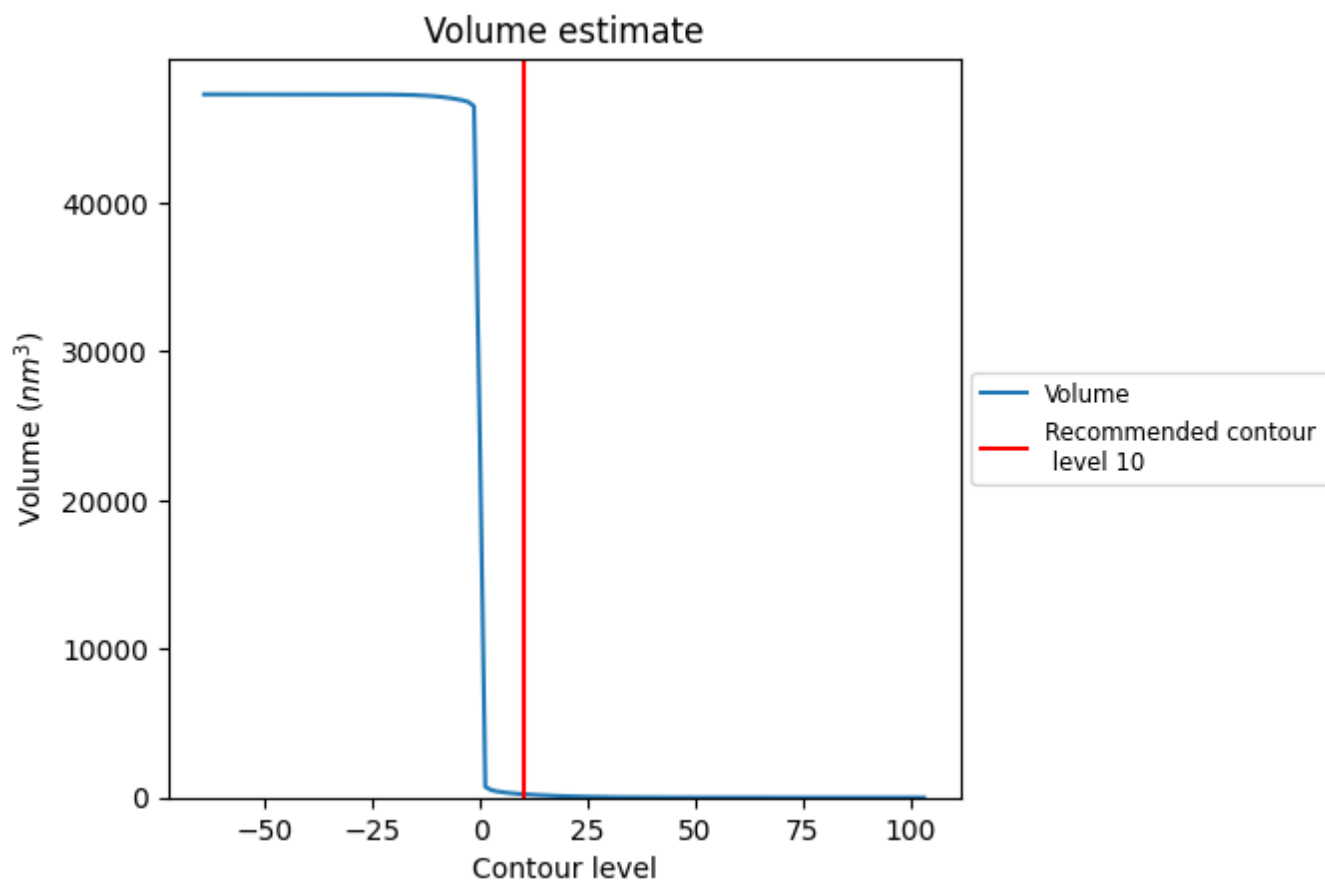
This section contains the results of statistical analysis of the map.

### 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.

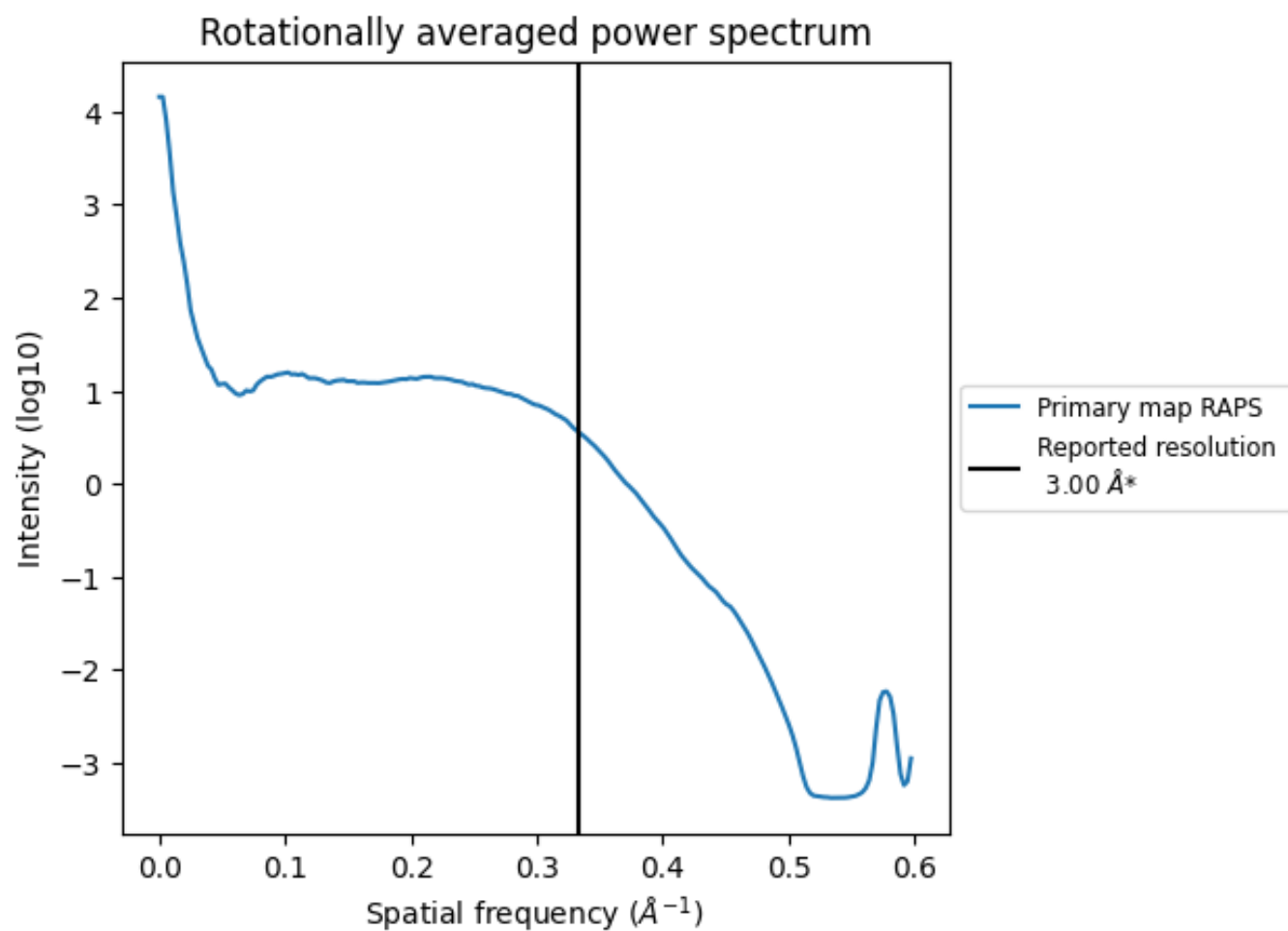
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229  $\text{nm}^3$ ; this corresponds to an approximate mass of 207 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 0.333 Å<sup>-1</sup>

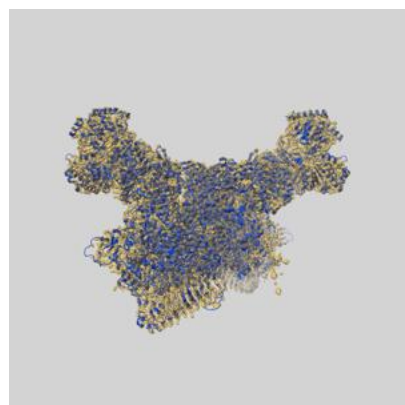
## 8 Fourier-Shell correlation

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

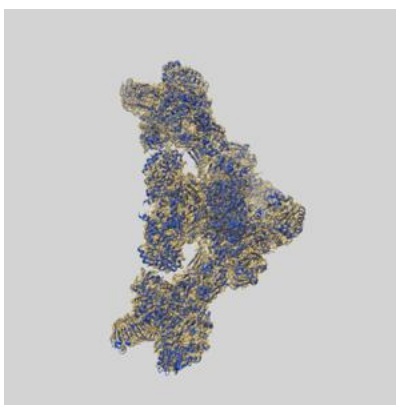
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12209 and PDB model 7BKC. Per-residue inclusion information can be found in section 3 on page 14.

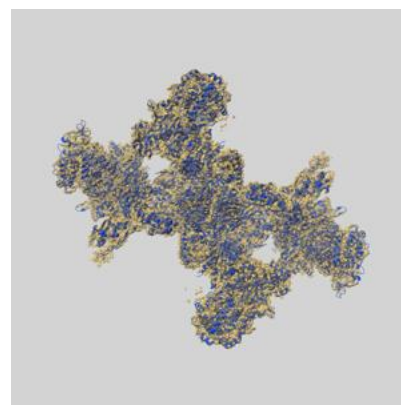
### 9.1 Map-model overlay [i](#)



X



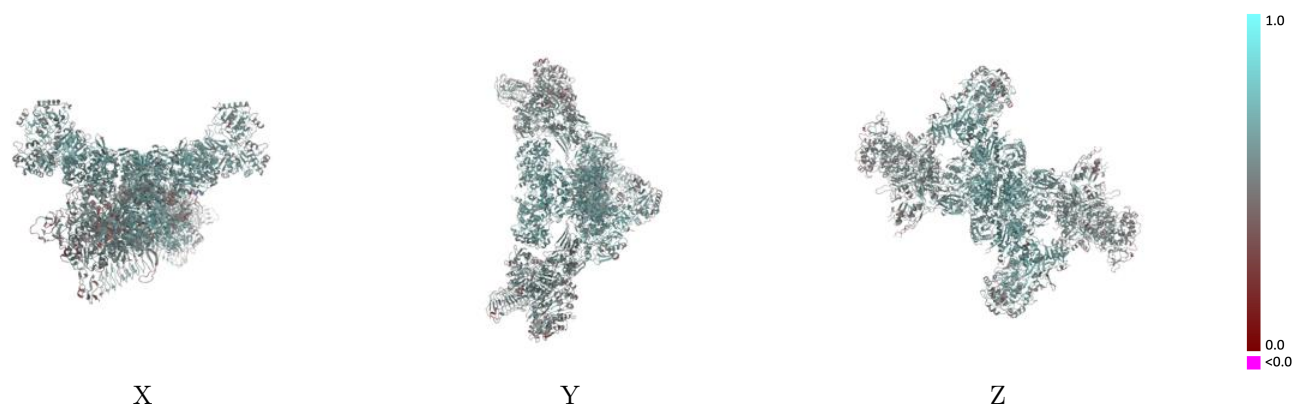
Y



Z

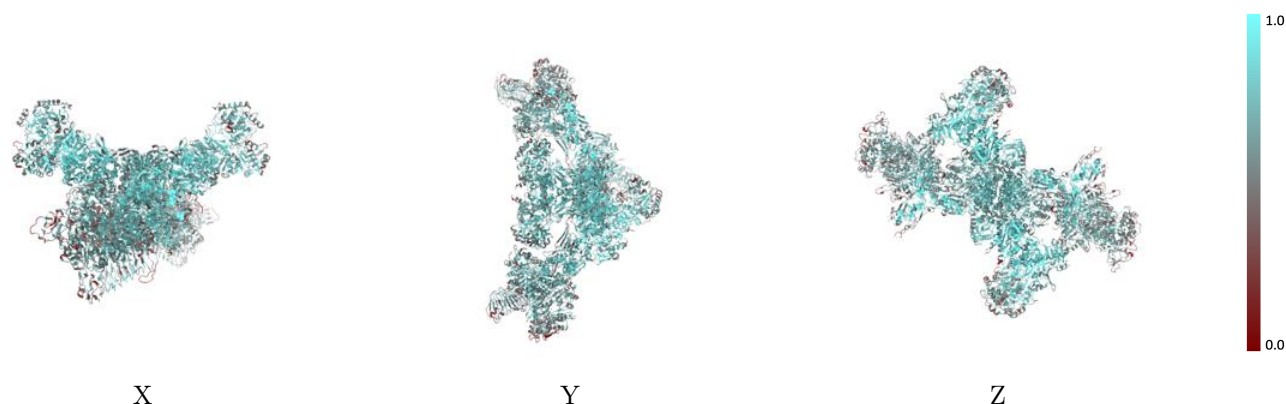
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



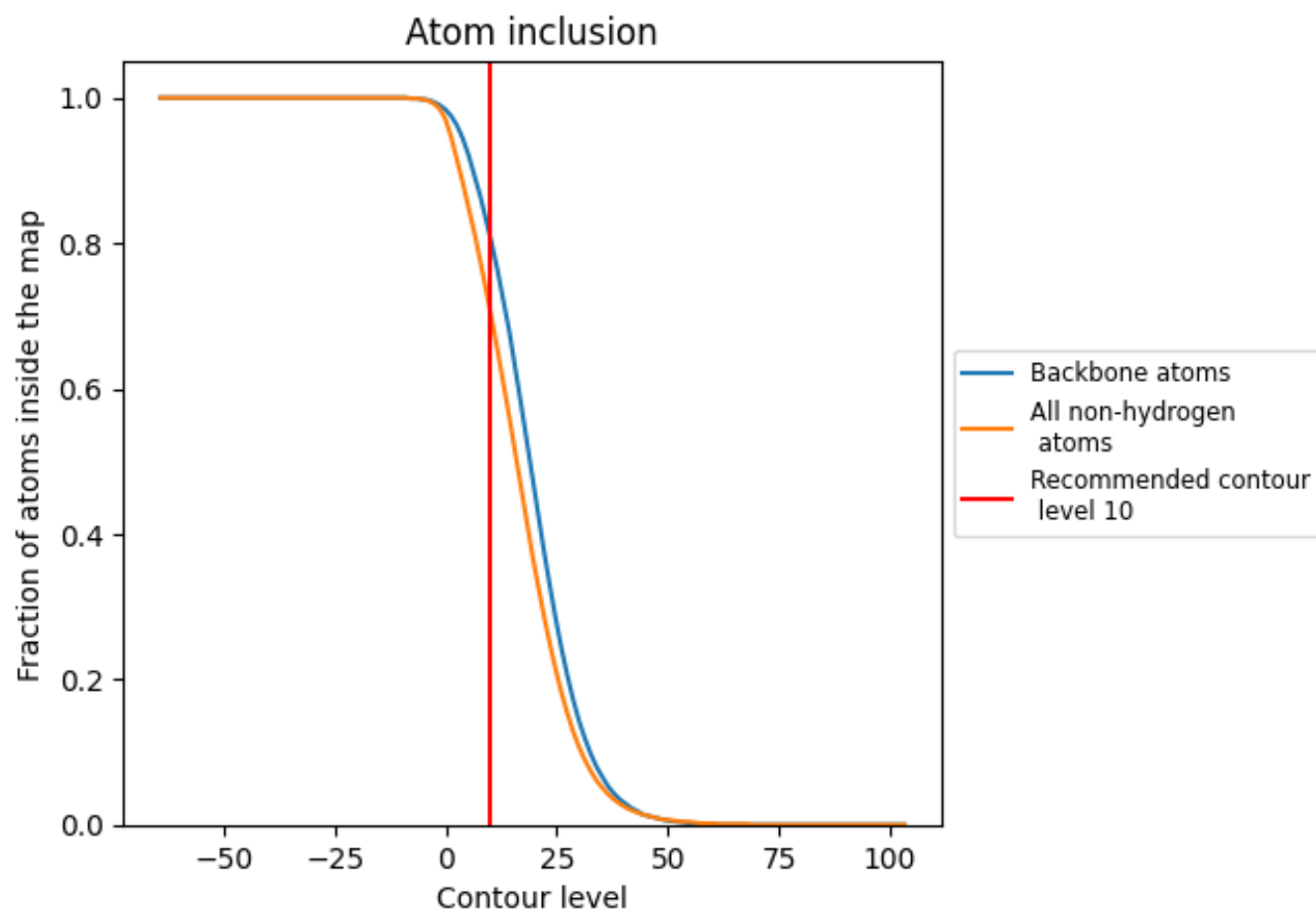
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (10) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7070   |  0.5690   |
| A     |  0.8180   |  0.6480   |
| B     |  0.7460   |  0.6300   |
| C     |  0.7510   |  0.6450   |
| D     |  0.6950   |  0.5610   |
| E     |  0.8240   |  0.6040   |
| F     |  0.8430   |  0.6230   |
| G     |  0.5790   |  0.4970   |
| H     |  0.6910   |  0.5390   |
| I     |  0.5380   |  0.4860   |
| J     |  0.6330   |  0.5310   |
| K     |  0.6600   |  0.5200   |
| L     |  0.7420   |  0.5590   |
| M     |  0.5990   |  0.4860   |
| a     |  0.8190  |  0.6460  |
| b     |  0.7440 |  0.6310 |
| c     |  0.7470 |  0.6420 |
| d     |  0.6930 |  0.5600 |
| e     |  0.8230 |  0.6050 |
| f     |  0.8460 |  0.6210 |
| g     |  0.5740 |  0.4980 |
| h     |  0.6960 |  0.5410 |
| i     |  0.5370 |  0.4850 |
| j     |  0.6340 |  0.5310 |
| k     |  0.6620 |  0.5200 |
| l     |  0.7470 |  0.5630 |
| m     |  0.6050 |  0.4880 |

