



## Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 04:14 am BST

PDB ID : 8QXT / pdb\_00008qxt  
EMDB ID : EMD-18736  
Title : CryoEM structure of a GroEL14-GroES7 complex in presence of ADP-BeFx with narrow GroEL7 trans ring conformation  
Authors : Wagner, J.; Caravajal, A.I.; Beck, F.; Bracher, A.; Wan, W.; Bohn, S.; Kerner, R.; Baumeister, W.; Fernandez-Busnadiego, R.; Hartl, F.U.  
Deposited on : 2023-10-25  
Resolution : 2.90 Å (reported)  
Based on initial models : 1SX3, 5OPX

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.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.50

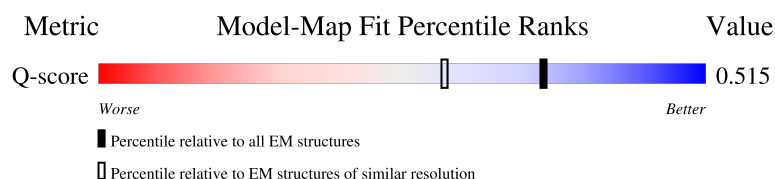
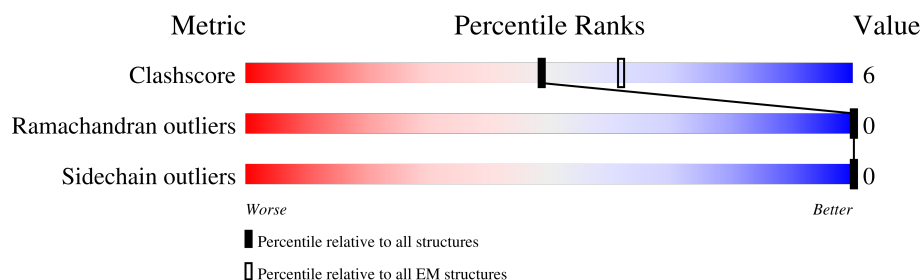
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | A     | 547    | <br>82% 14% . |
| 1   | B     | 547    | <br>84% 12% . |
| 1   | C     | 547    | <br>85% 11% . |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | D     | 547    |  82% 14% .   |
| 1   | E     | 547    |  84% 12% .   |
| 1   | F     | 547    |  85% 11% .   |
| 1   | G     | 547    |  80% 15% .   |
| 1   | H     | 547    |  82% 14% .   |
| 1   | I     | 547    |  84% 12% .   |
| 1   | J     | 547    |  84% 12% .   |
| 1   | K     | 547    |  82% 14% .   |
| 1   | L     | 547    |  80% 16% .   |
| 1   | M     | 547    |  83% 13% .   |
| 1   | N     | 547    |  82% 14% .   |
| 2   | O     | 97     |  77% 21% .  |
| 2   | P     | 97     |  85% 13% . |
| 2   | Q     | 97     |  82% 15% . |
| 2   | R     | 97     |  80% 18% . |
| 2   | S     | 97     |  78% 20% . |
| 2   | T     | 97     |  74% 24% . |
| 2   | U     | 97     |  77% 21% . |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5   | BEF  | C     | 1602 | -         | -        | X       | -                |
| 5   | BEF  | F     | 1602 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 59311 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 Chaperonin GroEL.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | B     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | C     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | D     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | E     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | F     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | G     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3851  | 2395 | 665 | 771 | 20 |         |       |
| 1   | H     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | I     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | J     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | K     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | L     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | M     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |
| 1   | N     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3864  | 2403 | 667 | 774 | 20 |         |       |

- Molecule 2 is a protein called Co-chaperonin GroES.

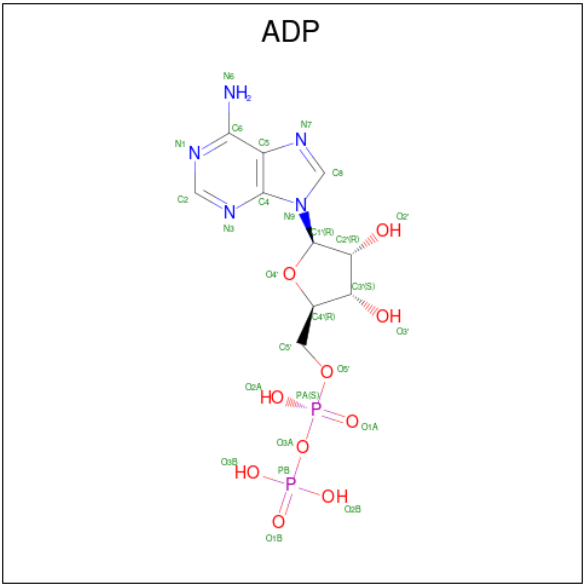
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | O     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | P     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |
| 2   | Q     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |
| 2   | R     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |
| 2   | S     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |
| 2   | T     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |
| 2   | U     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 430 | 125 | 131 | 1 |         |       |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 3   | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

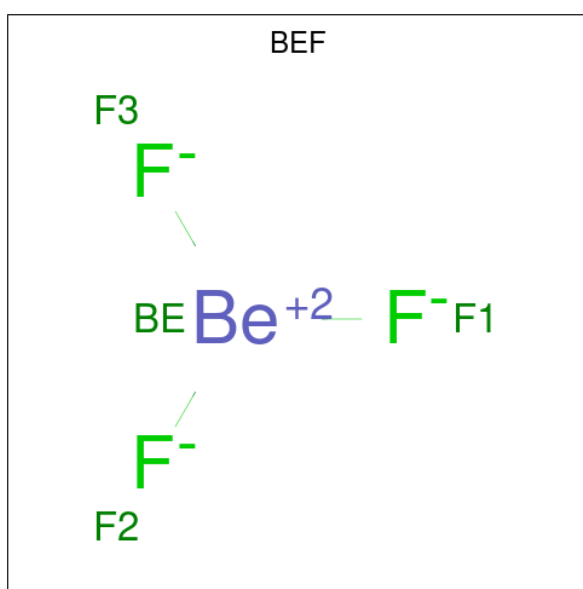
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | F     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | H     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | I     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | J     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | K     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | L     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | M     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | N     | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $\text{BeF}_3$ ).



| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 5   | A     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | B     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | C     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | D     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | E     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | F     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | G     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 6   | A     | 1        | Total K<br>1 1 | 0       |
| 6   | B     | 1        | Total K<br>1 1 | 0       |
| 6   | C     | 1        | Total K<br>1 1 | 0       |
| 6   | D     | 1        | Total K<br>1 1 | 0       |
| 6   | E     | 1        | Total K<br>1 1 | 0       |
| 6   | F     | 1        | Total K<br>1 1 | 0       |
| 6   | G     | 1        | Total K<br>1 1 | 0       |
| 6   | H     | 1        | Total K<br>1 1 | 0       |
| 6   | I     | 1        | Total K<br>1 1 | 0       |
| 6   | J     | 1        | Total K<br>1 1 | 0       |
| 6   | K     | 1        | Total K<br>1 1 | 0       |
| 6   | L     | 1        | Total K<br>1 1 | 0       |
| 6   | M     | 1        | Total K<br>1 1 | 0       |
| 6   | N     | 1        | Total K<br>1 1 | 0       |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 7   | A     | 6        | Total O<br>6 6 | 0       |
| 7   | B     | 6        | Total O<br>6 6 | 0       |
| 7   | C     | 6        | Total O<br>6 6 | 0       |
| 7   | D     | 6        | Total O<br>6 6 | 0       |
| 7   | E     | 6        | Total O<br>6 6 | 0       |

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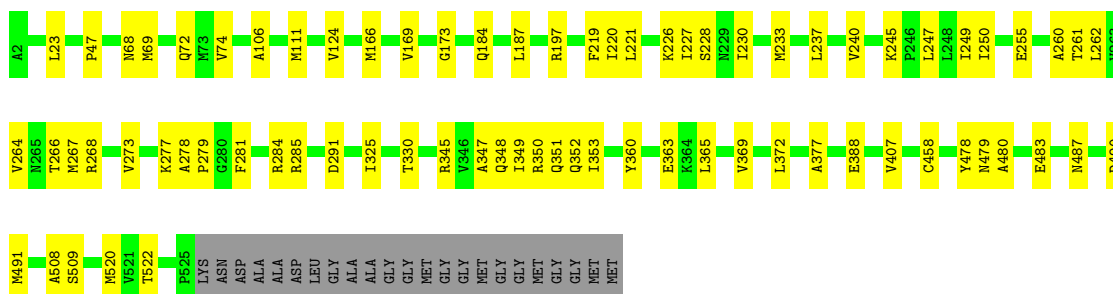
| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 7   | F     | 6        | Total<br>6 | O<br>6 | 0       |
| 7   | G     | 6        | Total<br>6 | O<br>6 | 0       |
| 7   | H     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | I     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | J     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | K     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | L     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | M     | 3        | Total<br>3 | O<br>3 | 0       |
| 7   | N     | 3        | Total<br>3 | O<br>3 | 0       |



MET  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
MET

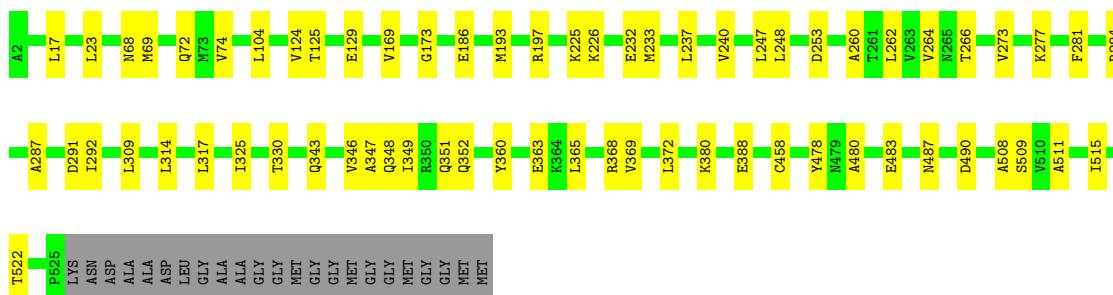
• Molecule 1: Chaperonin GroEL

Chain D:  82% 14%



• Molecule 1: Chaperonin GroEL

Chain E:  84% 12%



• Molecule 1: Chaperonin GroEL

Chain F:  85% 11%

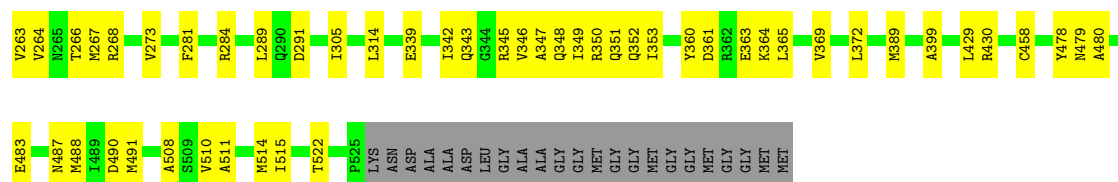


MET  
GLY  
GLY  
MET  
GLY  
GLY  
MET  
MET

• Molecule 1: Chaperonin GroEL

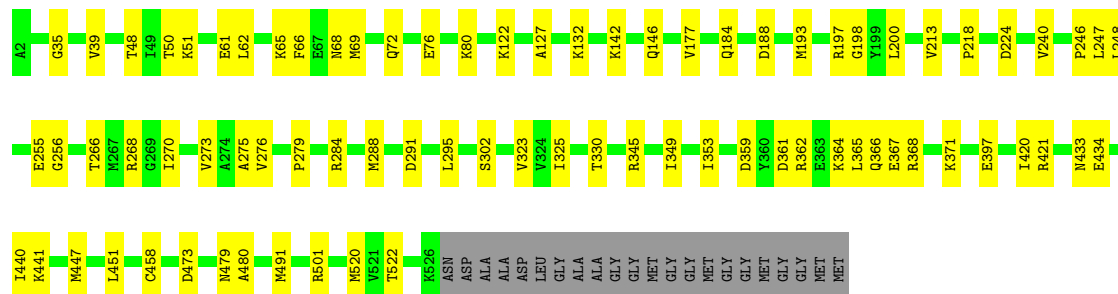
Chain G:  80% 15%





• Molecule 1: Chaperonin GroEL

Chain H: 82% 14% .



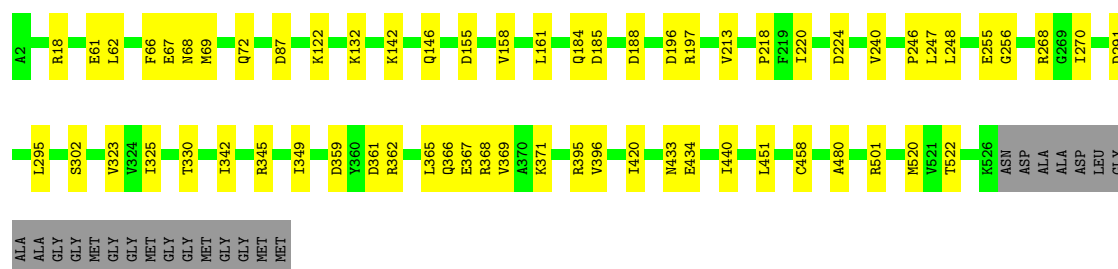
• Molecule 1: Chaperonin GroEL

Chain I: 84% 12% .



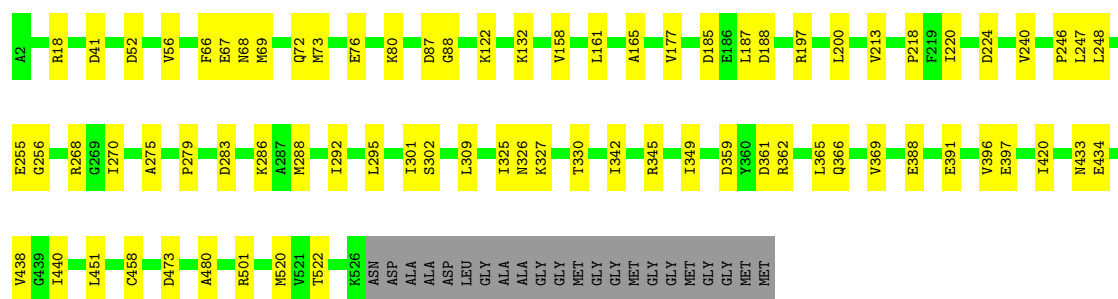
• Molecule 1: Chaperonin GroEL

Chain J: 84% 12% .



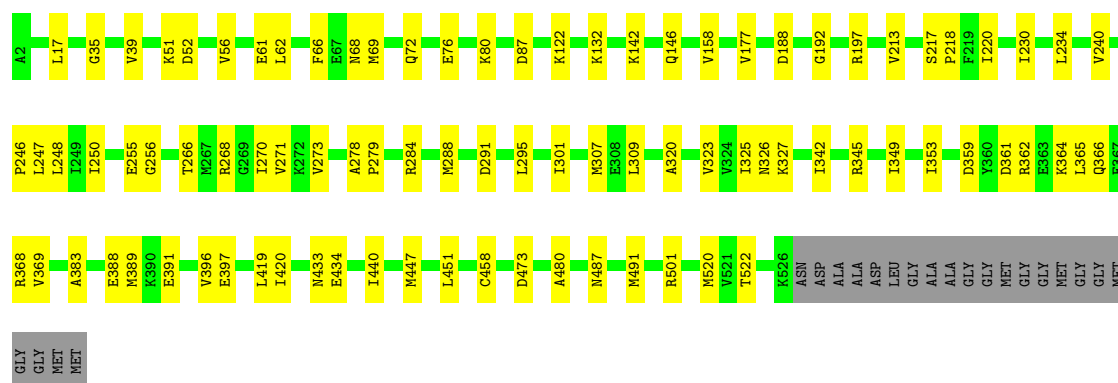
• Molecule 1: Chaperonin GroEL

Chain K: 82% 14% .



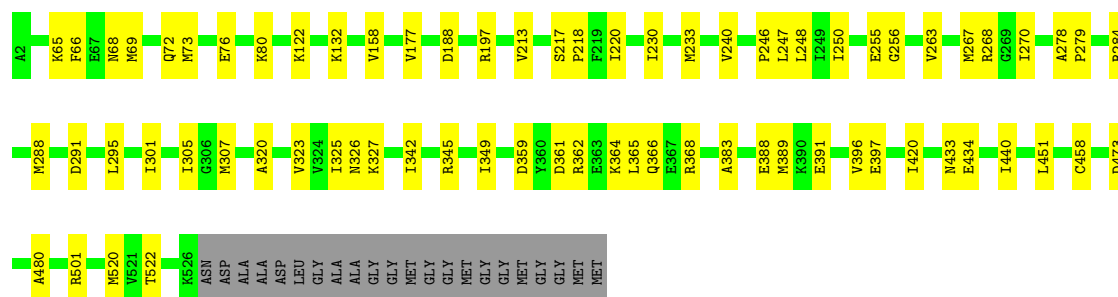
• Molecule 1: Chaperonin GroEL

Chain L: 80% 16% .



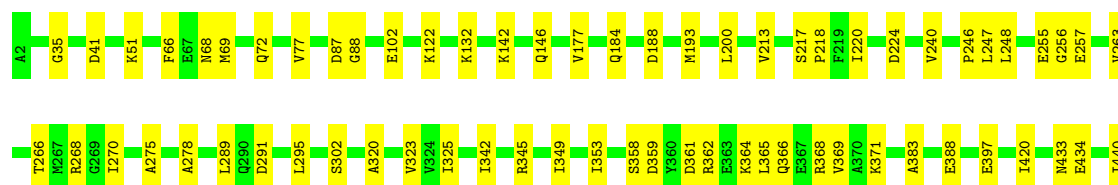
• Molecule 1: Chaperonin GroEL

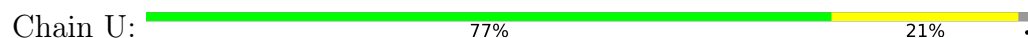
Chain M: 83% 13% .



• Molecule 1: Chaperonin GroEL

Chain N: 82% 14% .







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C7                               | Depositor |
| Number of particles used             | 169454                                  | 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 ( $e^-/\text{\AA}^2$ ) | 55                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 22500                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 7.595                                   | Depositor |
| Minimum map value                    | -3.380                                  | Depositor |
| Average map value                    | 0.006                                   | Depositor |
| Map value standard deviation         | 0.165                                   | Depositor |
| Recommended contour level            | 0.268                                   | Depositor |
| Map size (Å)                         | 353.16, 353.16, 353.16                  | wwPDB     |
| Map dimensions                       | 324, 324, 324                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.09, 1.09, 1.09                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.22         | 0/3879  | 0.37        | 0/5238  |
| 1   | B     | 0.22         | 0/3879  | 0.37        | 0/5238  |
| 1   | C     | 0.22         | 0/3879  | 0.34        | 0/5238  |
| 1   | D     | 0.22         | 0/3879  | 0.36        | 0/5238  |
| 1   | E     | 0.22         | 0/3879  | 0.35        | 0/5238  |
| 1   | F     | 0.22         | 0/3879  | 0.37        | 0/5238  |
| 1   | G     | 0.22         | 0/3879  | 0.38        | 0/5238  |
| 1   | H     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | I     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | J     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | K     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | L     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | M     | 0.18         | 0/3892  | 0.32        | 0/5254  |
| 1   | N     | 0.18         | 0/3892  | 0.33        | 0/5254  |
| 2   | O     | 0.13         | 0/690   | 0.33        | 0/930   |
| 2   | P     | 0.12         | 0/690   | 0.29        | 0/930   |
| 2   | Q     | 0.12         | 0/690   | 0.34        | 0/930   |
| 2   | R     | 0.13         | 0/690   | 0.34        | 0/930   |
| 2   | S     | 0.11         | 0/690   | 0.29        | 0/930   |
| 2   | T     | 0.12         | 0/690   | 0.31        | 0/930   |
| 2   | U     | 0.12         | 0/690   | 0.30        | 0/930   |
| All | All   | 0.20         | 0/59227 | 0.34        | 0/79954 |

There are no bond length outliers.

There are no bond angle outliers.

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     | 3851  | 0        | 3971     | 47      | 0            |
| 1   | B     | 3851  | 0        | 3971     | 40      | 0            |
| 1   | C     | 3851  | 0        | 3972     | 35      | 0            |
| 1   | D     | 3851  | 0        | 3972     | 46      | 0            |
| 1   | E     | 3851  | 0        | 3972     | 39      | 0            |
| 1   | F     | 3851  | 0        | 3972     | 36      | 0            |
| 1   | G     | 3851  | 0        | 3972     | 54      | 0            |
| 1   | H     | 3864  | 0        | 3989     | 50      | 0            |
| 1   | I     | 3864  | 0        | 3989     | 39      | 0            |
| 1   | J     | 3864  | 0        | 3989     | 39      | 0            |
| 1   | K     | 3864  | 0        | 3989     | 45      | 0            |
| 1   | L     | 3864  | 0        | 3989     | 55      | 0            |
| 1   | M     | 3864  | 0        | 3989     | 45      | 0            |
| 1   | N     | 3864  | 0        | 3989     | 47      | 0            |
| 2   | O     | 687   | 0        | 718      | 12      | 0            |
| 2   | P     | 687   | 0        | 718      | 7       | 0            |
| 2   | Q     | 687   | 0        | 718      | 9       | 0            |
| 2   | R     | 687   | 0        | 718      | 10      | 0            |
| 2   | S     | 687   | 0        | 718      | 11      | 0            |
| 2   | T     | 687   | 0        | 718      | 14      | 0            |
| 2   | U     | 687   | 0        | 718      | 12      | 0            |
| 3   | A     | 27    | 0        | 12       | 1       | 0            |
| 3   | B     | 27    | 0        | 12       | 1       | 0            |
| 3   | C     | 27    | 0        | 12       | 3       | 0            |
| 3   | D     | 27    | 0        | 12       | 2       | 0            |
| 3   | E     | 27    | 0        | 12       | 1       | 0            |
| 3   | F     | 27    | 0        | 12       | 2       | 0            |
| 3   | G     | 27    | 0        | 12       | 2       | 0            |
| 3   | H     | 27    | 0        | 12       | 1       | 0            |
| 3   | I     | 27    | 0        | 12       | 1       | 0            |
| 3   | J     | 27    | 0        | 12       | 1       | 0            |
| 3   | K     | 27    | 0        | 12       | 1       | 0            |
| 3   | L     | 27    | 0        | 12       | 1       | 0            |
| 3   | M     | 27    | 0        | 12       | 0       | 0            |
| 3   | N     | 27    | 0        | 12       | 1       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 1     | 0        | 0        | 0       | 0            |
| 4   | N     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 4     | 0        | 0        | 1       | 0            |
| 5   | B     | 4     | 0        | 0        | 0       | 0            |
| 5   | C     | 4     | 0        | 0        | 2       | 0            |
| 5   | D     | 4     | 0        | 0        | 1       | 0            |
| 5   | E     | 4     | 0        | 0        | 1       | 0            |
| 5   | F     | 4     | 0        | 0        | 2       | 0            |
| 5   | G     | 4     | 0        | 0        | 1       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 1     | 0        | 0        | 0       | 0            |
| 6   | I     | 1     | 0        | 0        | 0       | 0            |
| 6   | J     | 1     | 0        | 0        | 0       | 0            |
| 6   | K     | 1     | 0        | 0        | 0       | 0            |
| 6   | L     | 1     | 0        | 0        | 0       | 0            |
| 6   | M     | 1     | 0        | 0        | 0       | 0            |
| 6   | N     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 6     | 0        | 0        | 0       | 0            |
| 7   | B     | 6     | 0        | 0        | 1       | 0            |
| 7   | C     | 6     | 0        | 0        | 1       | 0            |
| 7   | D     | 6     | 0        | 0        | 1       | 0            |
| 7   | E     | 6     | 0        | 0        | 0       | 0            |
| 7   | F     | 6     | 0        | 0        | 0       | 0            |
| 7   | G     | 6     | 0        | 0        | 1       | 0            |
| 7   | H     | 3     | 0        | 0        | 1       | 0            |
| 7   | I     | 3     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | J     | 3     | 0        | 0        | 2       | 0            |
| 7   | K     | 3     | 0        | 0        | 1       | 0            |
| 7   | L     | 3     | 0        | 0        | 2       | 0            |
| 7   | M     | 3     | 0        | 0        | 0       | 0            |
| 7   | N     | 3     | 0        | 0        | 1       | 0            |
| All | All   | 59311 | 0        | 60919    | 694     | 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 6.

All (694) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:73:MET:HE3   | 1:G:514:MET:HE3  | 1.61                     | 0.82              |
| 1:F:240:VAL:HG21 | 1:F:247:LEU:HD12 | 1.61                     | 0.81              |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HD12 | 1.62                     | 0.81              |
| 1:A:227:ILE:HG21 | 1:A:233:MET:HE3  | 1.62                     | 0.80              |
| 1:B:69:MET:HE3   | 1:B:520:MET:HE2  | 1.62                     | 0.79              |
| 1:D:69:MET:HE2   | 1:D:522:THR:HB   | 1.67                     | 0.77              |
| 1:J:362:ARG:O    | 1:J:366:GLN:NE2  | 2.18                     | 0.76              |
| 1:L:362:ARG:O    | 1:L:366:GLN:NE2  | 2.19                     | 0.75              |
| 1:I:362:ARG:O    | 1:I:366:GLN:NE2  | 2.19                     | 0.75              |
| 1:E:69:MET:HE2   | 1:E:522:THR:HB   | 1.69                     | 0.74              |
| 1:H:479:ASN:HD22 | 1:H:491:MET:HE2  | 1.50                     | 0.74              |
| 1:K:362:ARG:O    | 1:K:366:GLN:NE2  | 2.18                     | 0.74              |
| 3:A:1600:ADP:PB  | 5:A:1602:BEF:F1  | 2.33                     | 0.74              |
| 1:A:240:VAL:HG21 | 1:A:247:LEU:HD12 | 1.68                     | 0.74              |
| 1:N:362:ARG:O    | 1:N:366:GLN:NE2  | 2.22                     | 0.73              |
| 1:M:220:ILE:HG22 | 1:M:248:LEU:HB3  | 1.71                     | 0.72              |
| 3:G:1600:ADP:PB  | 5:G:1602:BEF:F1  | 2.31                     | 0.72              |
| 1:A:321:LYS:HD3  | 1:A:322:ARG:HG3  | 1.69                     | 0.72              |
| 1:L:220:ILE:HG22 | 1:L:248:LEU:HB3  | 1.71                     | 0.72              |
| 3:E:1600:ADP:PB  | 5:E:1602:BEF:F1  | 2.31                     | 0.71              |
| 1:J:220:ILE:HG22 | 1:J:248:LEU:HB3  | 1.72                     | 0.71              |
| 2:S:11:ILE:HG12  | 2:S:85:ILE:HG12  | 1.72                     | 0.71              |
| 2:P:57:LEU:HD12  | 2:P:88:GLU:HG3   | 1.73                     | 0.71              |
| 1:B:321:LYS:HD3  | 1:B:322:ARG:HG3  | 1.72                     | 0.70              |
| 2:S:65:VAL:HG12  | 2:S:94:ILE:HG22  | 1.73                     | 0.70              |
| 2:O:11:ILE:HG12  | 2:O:85:ILE:HG12  | 1.74                     | 0.70              |
| 1:N:278:ALA:HB1  | 1:N:289:LEU:HD11 | 1.72                     | 0.70              |
| 3:C:1600:ADP:PB  | 5:C:1602:BEF:F1  | 2.38                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:40:LEU:HD22  | 1:F:59:GLU:HG2   | 1.74                     | 0.69              |
| 3:F:1600:ADP:PB  | 5:F:1602:BEF:F1  | 2.39                     | 0.69              |
| 1:N:433:ASN:OD1  | 1:N:434:GLU:N    | 2.25                     | 0.69              |
| 1:J:69:MET:HE3   | 1:J:522:THR:HB   | 1.74                     | 0.68              |
| 1:A:69:MET:HE3   | 1:A:520:MET:HE2  | 1.74                     | 0.68              |
| 3:D:1600:ADP:PB  | 5:D:1602:BEF:F1  | 2.33                     | 0.68              |
| 1:I:220:ILE:HG22 | 1:I:248:LEU:HB3  | 1.76                     | 0.68              |
| 2:T:11:ILE:HG12  | 2:T:85:ILE:HG12  | 1.74                     | 0.68              |
| 1:L:76:GLU:OE2   | 1:L:80:LYS:NZ    | 2.28                     | 0.67              |
| 1:B:240:VAL:HG11 | 1:B:247:LEU:HD12 | 1.76                     | 0.66              |
| 1:E:253:ASP:OD1  | 1:E:277:LYS:NZ   | 2.29                     | 0.66              |
| 1:J:213:VAL:HB   | 1:J:325:ILE:HB   | 1.78                     | 0.65              |
| 1:C:169:VAL:HG22 | 1:C:173:GLY:HA3  | 1.79                     | 0.65              |
| 1:N:220:ILE:HG22 | 1:N:248:LEU:HB3  | 1.78                     | 0.64              |
| 2:T:51:ASN:ND2   | 2:T:53:GLU:OE1   | 2.30                     | 0.64              |
| 1:F:339:GLU:O    | 1:F:343:GLN:NE2  | 2.31                     | 0.64              |
| 3:B:1600:ADP:O2A | 7:B:2001:HOH:O   | 2.15                     | 0.64              |
| 2:T:77:LYS:HE2   | 2:T:80:ASN:HA    | 1.79                     | 0.64              |
| 1:C:339:GLU:HB3  | 1:C:343:GLN:HE22 | 1.63                     | 0.64              |
| 1:F:339:GLU:HB3  | 1:F:343:GLN:HE22 | 1.62                     | 0.64              |
| 1:N:213:VAL:HB   | 1:N:325:ILE:HB   | 1.80                     | 0.63              |
| 1:N:291:ASP:OD2  | 1:N:368:ARG:NH1  | 2.32                     | 0.63              |
| 1:F:69:MET:HE2   | 1:F:522:THR:HB   | 1.81                     | 0.63              |
| 1:B:325:ILE:HG12 | 1:B:330:THR:HG23 | 1.80                     | 0.63              |
| 1:M:268:ARG:HG3  | 1:M:270:ILE:HG12 | 1.80                     | 0.63              |
| 2:S:76:GLU:HG3   | 2:S:78:ILE:HG23  | 1.80                     | 0.63              |
| 1:A:344:GLY:O    | 1:A:348:GLN:HG3  | 1.98                     | 0.62              |
| 1:D:325:ILE:HG12 | 1:D:330:THR:HG23 | 1.81                     | 0.62              |
| 1:A:169:VAL:HG22 | 1:A:173:GLY:HA3  | 1.82                     | 0.62              |
| 1:N:263:VAL:O    | 1:N:266:THR:OG1  | 2.13                     | 0.62              |
| 1:C:339:GLU:O    | 1:C:343:GLN:NE2  | 2.33                     | 0.62              |
| 1:K:213:VAL:HB   | 1:K:325:ILE:HB   | 1.82                     | 0.61              |
| 1:B:262:LEU:HD22 | 1:B:273:VAL:HG11 | 1.82                     | 0.61              |
| 1:K:268:ARG:HG3  | 1:K:270:ILE:HG12 | 1.83                     | 0.61              |
| 1:M:213:VAL:HB   | 1:M:325:ILE:HB   | 1.82                     | 0.61              |
| 1:D:233:MET:HB3  | 1:D:237:LEU:HD23 | 1.83                     | 0.61              |
| 1:E:225:LYS:NZ   | 1:E:232:GLU:OE1  | 2.32                     | 0.61              |
| 1:I:213:VAL:HB   | 1:I:325:ILE:HB   | 1.83                     | 0.61              |
| 1:H:65:LYS:O     | 1:H:69:MET:HG3   | 2.00                     | 0.60              |
| 2:R:47:ARG:NH1   | 2:R:88:GLU:OE2   | 2.33                     | 0.60              |
| 1:C:509:SER:OG   | 1:D:388:GLU:OE1  | 2.18                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:458:CYS:SG   | 1:H:480:ALA:HB1  | 2.41                     | 0.60              |
| 1:N:420:ILE:HD12 | 1:N:451:LEU:HD13 | 1.82                     | 0.60              |
| 1:G:69:MET:HE2   | 1:G:522:THR:HB   | 1.84                     | 0.60              |
| 1:H:213:VAL:HB   | 1:H:325:ILE:HB   | 1.84                     | 0.60              |
| 1:B:347:ALA:HA   | 1:B:350:ARG:HE   | 1.66                     | 0.59              |
| 1:K:366:GLN:HA   | 1:K:369:VAL:HG22 | 1.84                     | 0.59              |
| 1:J:66:PHE:HD1   | 1:J:520:MET:HE3  | 1.67                     | 0.59              |
| 1:J:268:ARG:HG3  | 1:J:270:ILE:HG12 | 1.84                     | 0.59              |
| 1:H:268:ARG:HG3  | 1:H:270:ILE:HG12 | 1.84                     | 0.59              |
| 1:K:220:ILE:HG22 | 1:K:248:LEU:HB3  | 1.85                     | 0.59              |
| 1:N:295:LEU:HA   | 1:N:342:ILE:HD11 | 1.85                     | 0.59              |
| 1:J:291:ASP:OD2  | 1:J:368:ARG:NH1  | 2.35                     | 0.59              |
| 1:B:281:PHE:HB2  | 1:B:284:ARG:HH21 | 1.66                     | 0.59              |
| 1:C:228:SER:HA   | 1:C:255:GLU:HB2  | 1.85                     | 0.59              |
| 1:L:35:GLY:O     | 1:L:51:LYS:NZ    | 2.32                     | 0.59              |
| 1:E:478:TYR:OH   | 1:E:483:GLU:OE1  | 2.20                     | 0.58              |
| 1:I:66:PHE:HD1   | 1:I:520:MET:HE3  | 1.68                     | 0.58              |
| 1:M:248:LEU:HD22 | 1:M:323:VAL:HG11 | 1.86                     | 0.58              |
| 1:J:142:LYS:O    | 1:J:146:GLN:HG2  | 2.02                     | 0.58              |
| 1:L:420:ILE:HD12 | 1:L:451:LEU:HD13 | 1.84                     | 0.58              |
| 1:K:288:MET:O    | 1:K:292:ILE:HD12 | 2.03                     | 0.58              |
| 1:L:248:LEU:HD22 | 1:L:323:VAL:HG11 | 1.85                     | 0.58              |
| 2:P:65:VAL:HG12  | 2:P:94:ILE:HG22  | 1.85                     | 0.58              |
| 1:G:40:LEU:HD22  | 1:G:59:GLU:HG2   | 1.85                     | 0.58              |
| 1:G:226:LYS:HZ1  | 1:G:255:GLU:HG2  | 1.68                     | 0.58              |
| 1:M:420:ILE:HD12 | 1:M:451:LEU:HD13 | 1.85                     | 0.58              |
| 1:J:420:ILE:HD12 | 1:J:451:LEU:HD13 | 1.84                     | 0.58              |
| 1:N:248:LEU:HD22 | 1:N:323:VAL:HG11 | 1.86                     | 0.58              |
| 1:A:73:MET:HE3   | 1:A:514:MET:HE3  | 1.86                     | 0.58              |
| 1:B:226:LYS:HZ1  | 1:B:255:GLU:HG2  | 1.69                     | 0.58              |
| 1:H:420:ILE:HD12 | 1:H:451:LEU:HD13 | 1.85                     | 0.58              |
| 1:J:161:LEU:HD11 | 1:J:185:ASP:HB3  | 1.86                     | 0.58              |
| 1:M:69:MET:O     | 1:M:73:MET:HG3   | 2.03                     | 0.58              |
| 1:B:365:LEU:O    | 1:B:369:VAL:HG23 | 2.03                     | 0.58              |
| 1:M:65:LYS:O     | 1:M:69:MET:HG3   | 2.04                     | 0.58              |
| 1:N:142:LYS:O    | 1:N:146:GLN:HG2  | 2.04                     | 0.57              |
| 1:N:240:VAL:HG21 | 1:N:247:LEU:HD22 | 1.85                     | 0.57              |
| 1:I:366:GLN:HA   | 1:I:369:VAL:HG22 | 1.85                     | 0.57              |
| 1:I:420:ILE:HD12 | 1:I:451:LEU:HD13 | 1.85                     | 0.57              |
| 1:G:345:ARG:O    | 1:G:349:ILE:HG13 | 2.04                     | 0.57              |
| 1:J:248:LEU:HD22 | 1:J:323:VAL:HG11 | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:420:ILE:HD12 | 1:K:451:LEU:HD13 | 1.85                     | 0.57              |
| 1:F:262:LEU:HD22 | 1:F:273:VAL:HG11 | 1.86                     | 0.57              |
| 1:L:361:ASP:HA   | 1:L:364:LYS:HE3  | 1.87                     | 0.57              |
| 1:A:234:LEU:O    | 1:A:238:GLU:HG3  | 2.04                     | 0.57              |
| 1:M:458:CYS:SG   | 1:M:480:ALA:HB1  | 2.44                     | 0.57              |
| 1:N:458:CYS:SG   | 1:N:480:ALA:HB1  | 2.45                     | 0.57              |
| 1:I:248:LEU:HD22 | 1:I:323:VAL:HG11 | 1.86                     | 0.56              |
| 1:A:262:LEU:HD22 | 1:A:273:VAL:HG11 | 1.87                     | 0.56              |
| 1:D:219:PHE:HE2  | 1:D:245:LYS:HG3  | 1.71                     | 0.56              |
| 1:N:383:ALA:HB1  | 1:N:388:GLU:HG3  | 1.86                     | 0.56              |
| 1:F:281:PHE:H    | 1:F:284:ARG:HE   | 1.53                     | 0.56              |
| 1:L:366:GLN:HA   | 1:L:369:VAL:HG22 | 1.87                     | 0.56              |
| 1:D:350:ARG:HA   | 1:D:353:ILE:HD12 | 1.87                     | 0.56              |
| 1:G:262:LEU:HD22 | 1:G:273:VAL:HG11 | 1.86                     | 0.56              |
| 1:I:458:CYS:SG   | 1:I:480:ALA:HB1  | 2.46                     | 0.56              |
| 1:K:388:GLU:HA   | 1:K:391:GLU:HG2  | 1.87                     | 0.56              |
| 1:N:66:PHE:HD1   | 1:N:520:MET:HE3  | 1.70                     | 0.56              |
| 1:C:350:ARG:HA   | 1:C:353:ILE:HD12 | 1.88                     | 0.56              |
| 1:F:69:MET:HE3   | 1:F:520:MET:HE2  | 1.88                     | 0.56              |
| 1:K:240:VAL:HG21 | 1:K:247:LEU:HD22 | 1.88                     | 0.56              |
| 1:D:262:LEU:HD22 | 1:D:273:VAL:HG11 | 1.88                     | 0.56              |
| 1:D:291:ASP:HB3  | 1:D:372:LEU:HD21 | 1.87                     | 0.56              |
| 1:K:458:CYS:SG   | 1:K:480:ALA:HB1  | 2.45                     | 0.56              |
| 1:L:142:LYS:O    | 1:L:146:GLN:HG2  | 2.05                     | 0.56              |
| 1:D:478:TYR:OH   | 1:D:483:GLU:OE1  | 2.23                     | 0.56              |
| 1:L:383:ALA:HB1  | 1:L:388:GLU:HG3  | 1.88                     | 0.56              |
| 1:A:291:ASP:HB3  | 1:A:372:LEU:HD21 | 1.87                     | 0.56              |
| 1:B:478:TYR:OH   | 1:B:483:GLU:OE1  | 2.24                     | 0.56              |
| 1:E:262:LEU:HD22 | 1:E:273:VAL:HG11 | 1.86                     | 0.56              |
| 1:H:240:VAL:HG21 | 1:H:247:LEU:HD22 | 1.86                     | 0.56              |
| 1:K:66:PHE:HD1   | 1:K:520:MET:HE3  | 1.71                     | 0.56              |
| 1:G:361:ASP:O    | 1:G:365:LEU:HG   | 2.06                     | 0.56              |
| 1:J:458:CYS:SG   | 1:J:480:ALA:HB1  | 2.46                     | 0.56              |
| 1:L:458:CYS:SG   | 1:L:480:ALA:HB1  | 2.46                     | 0.56              |
| 1:I:240:VAL:HG21 | 1:I:247:LEU:HD22 | 1.87                     | 0.55              |
| 1:C:478:TYR:OH   | 1:C:483:GLU:OE1  | 2.24                     | 0.55              |
| 1:L:268:ARG:HG3  | 1:L:270:ILE:HG12 | 1.87                     | 0.55              |
| 1:L:213:VAL:HB   | 1:L:325:ILE:HB   | 1.88                     | 0.55              |
| 1:D:197:ARG:O    | 1:D:330:THR:OG1  | 2.24                     | 0.55              |
| 1:J:366:GLN:HA   | 1:J:369:VAL:HG22 | 1.87                     | 0.55              |
| 1:M:388:GLU:HA   | 1:M:391:GLU:HG2  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:478:TYR:OH   | 1:G:483:GLU:OE1  | 2.24                     | 0.55              |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:HD12 | 1.89                     | 0.55              |
| 1:B:487:ASN:ND2  | 1:B:490:ASP:OD2  | 2.40                     | 0.55              |
| 3:G:1600:ADP:O2A | 7:G:2001:HOH:O   | 2.18                     | 0.54              |
| 1:H:142:LYS:O    | 1:H:146:GLN:HG2  | 2.07                     | 0.54              |
| 1:L:122:LYS:HD3  | 1:L:440:ILE:HD11 | 1.89                     | 0.54              |
| 1:L:66:PHE:HD1   | 1:L:520:MET:HE3  | 1.73                     | 0.54              |
| 1:M:359:ASP:OD1  | 1:M:362:ARG:NH1  | 2.40                     | 0.54              |
| 1:B:236:VAL:HG23 | 1:B:237:LEU:HD12 | 1.89                     | 0.54              |
| 1:H:291:ASP:OD2  | 1:H:368:ARG:NH1  | 2.40                     | 0.54              |
| 1:K:69:MET:HE2   | 1:K:522:THR:HB   | 1.89                     | 0.54              |
| 1:C:262:LEU:HD22 | 1:C:273:VAL:HG11 | 1.88                     | 0.54              |
| 1:J:359:ASP:OD1  | 1:J:362:ARG:NH1  | 2.39                     | 0.54              |
| 1:A:228:SER:HA   | 1:A:255:GLU:HB2  | 1.90                     | 0.54              |
| 1:I:69:MET:HE2   | 1:I:522:THR:HB   | 1.90                     | 0.54              |
| 1:G:365:LEU:O    | 1:G:369:VAL:HG23 | 2.08                     | 0.54              |
| 3:H:601:ADP:O1B  | 7:H:701:HOH:O    | 2.18                     | 0.54              |
| 1:D:365:LEU:O    | 1:D:369:VAL:HG23 | 2.08                     | 0.54              |
| 1:J:295:LEU:HA   | 1:J:342:ILE:HD11 | 1.89                     | 0.54              |
| 1:L:68:ASN:O     | 1:L:72:GLN:HG2   | 2.08                     | 0.54              |
| 1:M:349:ILE:HG23 | 1:M:365:LEU:HD12 | 1.90                     | 0.54              |
| 1:H:66:PHE:HD1   | 1:H:520:MET:HE3  | 1.73                     | 0.53              |
| 2:R:73:VAL:HG12  | 2:R:84:LEU:HD12  | 1.90                     | 0.53              |
| 1:J:122:LYS:HD3  | 1:J:440:ILE:HD11 | 1.91                     | 0.53              |
| 1:H:193:MET:HE2  | 1:H:295:LEU:HD22 | 1.90                     | 0.53              |
| 1:N:366:GLN:HA   | 1:N:369:VAL:HG22 | 1.90                     | 0.53              |
| 3:C:1600:ADP:O2A | 7:C:2001:HOH:O   | 2.19                     | 0.53              |
| 1:G:228:SER:HA   | 1:G:255:GLU:HB2  | 1.90                     | 0.53              |
| 1:L:132:LYS:NZ   | 1:L:501:ARG:HD3  | 2.24                     | 0.53              |
| 1:L:295:LEU:HA   | 1:L:342:ILE:HD11 | 1.90                     | 0.53              |
| 1:M:66:PHE:HD1   | 1:M:520:MET:HE3  | 1.73                     | 0.53              |
| 1:B:226:LYS:NZ   | 1:B:255:GLU:HG2  | 2.22                     | 0.53              |
| 1:G:350:ARG:HA   | 1:G:353:ILE:HD12 | 1.90                     | 0.53              |
| 1:D:281:PHE:H    | 1:D:284:ARG:HE   | 1.56                     | 0.53              |
| 1:E:365:LEU:O    | 1:E:369:VAL:HG23 | 2.09                     | 0.53              |
| 1:F:228:SER:HA   | 1:F:255:GLU:HB2  | 1.89                     | 0.53              |
| 1:G:240:VAL:HG21 | 1:G:247:LEU:HD12 | 1.90                     | 0.53              |
| 1:N:77:VAL:HG21  | 1:N:510:VAL:HB   | 1.91                     | 0.53              |
| 2:R:5:PRO:HD3    | 2:R:42:ALA:HB1   | 1.90                     | 0.53              |
| 1:B:73:MET:HE3   | 1:B:514:MET:HE3  | 1.91                     | 0.53              |
| 1:E:233:MET:HB3  | 1:E:237:LEU:HD23 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:U:11:ILE:HG12  | 2:U:85:ILE:HG13  | 1.90                     | 0.52              |
| 1:C:365:LEU:O    | 1:C:369:VAL:HG23 | 2.08                     | 0.52              |
| 1:I:359:ASP:OD1  | 1:I:362:ARG:NH1  | 2.40                     | 0.52              |
| 1:N:359:ASP:OD1  | 1:N:362:ARG:NH1  | 2.42                     | 0.52              |
| 2:Q:68:ASN:HB3   | 2:R:74:LYS:HE2   | 1.90                     | 0.52              |
| 2:R:68:ASN:HB3   | 2:S:74:LYS:HE2   | 1.91                     | 0.52              |
| 1:D:345:ARG:O    | 1:D:349:ILE:HG13 | 2.09                     | 0.52              |
| 1:H:349:ILE:HG23 | 1:H:365:LEU:HD12 | 1.90                     | 0.52              |
| 1:F:205:ILE:HA   | 1:F:213:VAL:HG22 | 1.90                     | 0.52              |
| 1:N:132:LYS:NZ   | 1:N:501:ARG:HD3  | 2.24                     | 0.52              |
| 1:D:197:ARG:HD3  | 1:D:277:LYS:HB2  | 1.90                     | 0.52              |
| 1:F:188:ASP:OD2  | 1:F:380:LYS:NZ   | 2.35                     | 0.52              |
| 1:G:291:ASP:HB3  | 1:G:372:LEU:HD21 | 1.91                     | 0.52              |
| 1:K:68:ASN:O     | 1:K:72:GLN:HG2   | 2.08                     | 0.52              |
| 2:O:5:PRO:HD3    | 2:O:42:ALA:HB1   | 1.91                     | 0.52              |
| 1:I:68:ASN:O     | 1:I:72:GLN:HG2   | 2.09                     | 0.52              |
| 1:I:122:LYS:HD3  | 1:I:440:ILE:HD11 | 1.91                     | 0.52              |
| 1:L:69:MET:CE    | 1:L:522:THR:HB   | 2.40                     | 0.52              |
| 2:T:5:PRO:HD3    | 2:T:42:ALA:HB1   | 1.91                     | 0.52              |
| 1:N:87:ASP:OD1   | 1:N:88:GLY:N     | 2.42                     | 0.52              |
| 2:Q:65:VAL:HG12  | 2:Q:94:ILE:HG22  | 1.92                     | 0.52              |
| 1:B:197:ARG:O    | 1:B:330:THR:OG1  | 2.27                     | 0.52              |
| 1:H:255:GLU:OE1  | 1:H:256:GLY:N    | 2.43                     | 0.51              |
| 1:M:301:ILE:HG23 | 1:M:307:MET:HG2  | 1.92                     | 0.51              |
| 1:M:433:ASN:OD1  | 1:M:434:GLU:N    | 2.43                     | 0.51              |
| 1:M:383:ALA:HB1  | 1:M:388:GLU:HG3  | 1.92                     | 0.51              |
| 1:N:122:LYS:HD3  | 1:N:440:ILE:HD11 | 1.92                     | 0.51              |
| 1:D:487:ASN:ND2  | 1:D:490:ASP:OD2  | 2.42                     | 0.51              |
| 1:K:132:LYS:NZ   | 1:K:501:ARG:HD3  | 2.24                     | 0.51              |
| 1:K:433:ASN:OD1  | 1:K:434:GLU:N    | 2.43                     | 0.51              |
| 1:A:478:TYR:OH   | 1:A:483:GLU:OE1  | 2.27                     | 0.51              |
| 1:M:284:ARG:HG2  | 1:M:288:MET:HE2  | 1.92                     | 0.51              |
| 1:A:203:TYR:CD1  | 1:G:305:ILE:HD13 | 2.46                     | 0.51              |
| 1:E:291:ASP:HB3  | 1:E:372:LEU:HD21 | 1.93                     | 0.51              |
| 1:H:68:ASN:O     | 1:H:72:GLN:HG2   | 2.09                     | 0.51              |
| 1:L:87:ASP:OD2   | 7:L:801:HOH:O    | 2.18                     | 0.51              |
| 1:L:433:ASN:OD1  | 1:L:434:GLU:N    | 2.43                     | 0.51              |
| 1:N:68:ASN:O     | 1:N:72:GLN:HG2   | 2.09                     | 0.51              |
| 2:U:5:PRO:HD3    | 2:U:42:ALA:HB1   | 1.91                     | 0.51              |
| 1:A:487:ASN:HB3  | 1:A:490:ASP:HB2  | 1.91                     | 0.51              |
| 1:D:23:LEU:HD22  | 1:D:74:VAL:HG13  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:39:VAL:HG12  | 1:N:69:MET:HE2   | 1.92                     | 0.51              |
| 1:I:291:ASP:OD2  | 1:I:368:ARG:NH1  | 2.43                     | 0.51              |
| 1:E:281:PHE:H    | 1:E:284:ARG:HE   | 1.59                     | 0.51              |
| 1:D:166:MET:HE1  | 1:D:407:VAL:HG21 | 1.93                     | 0.51              |
| 1:H:35:GLY:O     | 1:H:51:LYS:NZ    | 2.37                     | 0.51              |
| 2:R:40:VAL:HG23  | 2:R:62:GLY:H     | 1.76                     | 0.51              |
| 1:F:365:LEU:O    | 1:F:369:VAL:HG23 | 2.12                     | 0.50              |
| 1:E:314:LEU:HD13 | 1:E:317:LEU:HD12 | 1.93                     | 0.50              |
| 3:F:1600:ADP:O1B | 5:F:1602:BEF:F1  | 2.19                     | 0.50              |
| 1:M:68:ASN:O     | 1:M:72:GLN:HG2   | 2.11                     | 0.50              |
| 1:A:40:LEU:HD22  | 1:A:59:GLU:HG3   | 1.92                     | 0.50              |
| 1:A:487:ASN:ND2  | 1:A:490:ASP:OD1  | 2.28                     | 0.50              |
| 2:U:51:ASN:OD1   | 2:U:52:GLY:N     | 2.45                     | 0.50              |
| 2:U:73:VAL:HG12  | 2:U:84:LEU:HD12  | 1.93                     | 0.50              |
| 1:I:132:LYS:NZ   | 1:I:501:ARG:HD3  | 2.26                     | 0.50              |
| 1:L:240:VAL:HG21 | 1:L:247:LEU:HD22 | 1.93                     | 0.50              |
| 1:M:240:VAL:HG21 | 1:M:247:LEU:HD22 | 1.92                     | 0.50              |
| 1:M:255:GLU:OE1  | 1:M:256:GLY:N    | 2.45                     | 0.50              |
| 2:Q:12:VAL:HG12  | 2:Q:40:VAL:HG12  | 1.92                     | 0.50              |
| 1:A:39:VAL:HG22  | 1:A:49:ILE:HG12  | 1.93                     | 0.50              |
| 1:G:69:MET:O     | 1:G:73:MET:HG3   | 2.12                     | 0.50              |
| 1:H:359:ASP:OD1  | 1:H:362:ARG:NH1  | 2.42                     | 0.50              |
| 1:J:132:LYS:NZ   | 1:J:501:ARG:HD3  | 2.26                     | 0.50              |
| 1:K:73:MET:HE2   | 1:L:39:VAL:HG11  | 1.94                     | 0.50              |
| 1:N:193:MET:HG3  | 1:N:371:LYS:HG2  | 1.94                     | 0.50              |
| 2:P:5:PRO:HD3    | 2:P:42:ALA:HB1   | 1.93                     | 0.50              |
| 1:K:359:ASP:OD1  | 1:K:362:ARG:NH1  | 2.43                     | 0.49              |
| 1:F:478:TYR:OH   | 1:F:483:GLU:OE1  | 2.28                     | 0.49              |
| 1:K:295:LEU:HA   | 1:K:342:ILE:HD11 | 1.94                     | 0.49              |
| 1:M:122:LYS:HD3  | 1:M:440:ILE:HD11 | 1.94                     | 0.49              |
| 1:N:255:GLU:OE1  | 1:N:256:GLY:N    | 2.44                     | 0.49              |
| 1:M:345:ARG:O    | 1:M:349:ILE:HD12 | 2.13                     | 0.49              |
| 1:N:268:ARG:HG3  | 1:N:270:ILE:HG12 | 1.93                     | 0.49              |
| 1:C:267:MET:SD   | 1:C:268:ARG:HG2  | 2.53                     | 0.49              |
| 1:E:343:GLN:HA   | 1:E:346:VAL:HG22 | 1.95                     | 0.49              |
| 1:F:349:ILE:HA   | 1:F:352:GLN:CD   | 2.38                     | 0.49              |
| 1:L:301:ILE:HG23 | 1:L:307:MET:HG2  | 1.93                     | 0.49              |
| 1:M:291:ASP:OD2  | 1:M:368:ARG:NH1  | 2.45                     | 0.49              |
| 2:S:5:PRO:HD3    | 2:S:42:ALA:HB1   | 1.95                     | 0.49              |
| 1:D:360:TYR:O    | 1:D:363:GLU:HG3  | 2.13                     | 0.49              |
| 1:H:248:LEU:HD22 | 1:H:323:VAL:HG11 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:68:ASN:O     | 1:J:72:GLN:HG2   | 2.13                     | 0.49              |
| 1:L:255:GLU:OE1  | 1:L:256:GLY:N    | 2.46                     | 0.49              |
| 1:B:284:ARG:O    | 1:B:288:MET:HG3  | 2.12                     | 0.49              |
| 1:B:509:SER:OG   | 1:C:388:GLU:OE1  | 2.29                     | 0.49              |
| 1:J:255:GLU:OE1  | 1:J:256:GLY:N    | 2.45                     | 0.49              |
| 2:Q:6:LEU:HG     | 2:Q:7:HIS:CD2    | 2.47                     | 0.49              |
| 1:C:345:ARG:O    | 1:C:349:ILE:HG13 | 2.12                     | 0.49              |
| 1:G:488:MET:HE2  | 1:G:488:MET:HA   | 1.95                     | 0.49              |
| 1:D:240:VAL:HG11 | 1:D:247:LEU:HB2  | 1.95                     | 0.49              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:HB2  | 1.95                     | 0.49              |
| 1:L:230:ILE:O    | 1:L:234:LEU:HG   | 2.13                     | 0.49              |
| 1:M:326:ASN:OD1  | 1:M:327:LYS:N    | 2.42                     | 0.49              |
| 1:N:102:GLU:OE1  | 1:N:445:ARG:NH1  | 2.46                     | 0.49              |
| 1:G:267:MET:SD   | 1:G:268:ARG:HG2  | 2.53                     | 0.49              |
| 3:N:601:ADP:O1B  | 7:N:701:HOH:O    | 2.20                     | 0.49              |
| 1:G:233:MET:HG2  | 1:G:237:LEU:HD23 | 1.94                     | 0.48              |
| 1:G:253:ASP:OD1  | 1:G:254:VAL:N    | 2.46                     | 0.48              |
| 1:J:66:PHE:CD1   | 1:J:520:MET:HE3  | 2.48                     | 0.48              |
| 1:J:87:ASP:OD2   | 7:J:801:HOH:O    | 2.20                     | 0.48              |
| 1:M:295:LEU:HA   | 1:M:342:ILE:HD11 | 1.95                     | 0.48              |
| 1:N:218:PRO:HB3  | 1:N:246:PRO:HG2  | 1.95                     | 0.48              |
| 2:R:11:ILE:HG12  | 2:R:85:ILE:HG13  | 1.94                     | 0.48              |
| 1:H:284:ARG:O    | 1:H:288:MET:HG2  | 2.13                     | 0.48              |
| 1:K:218:PRO:HB3  | 1:K:246:PRO:HG2  | 1.95                     | 0.48              |
| 1:M:132:LYS:NZ   | 1:M:501:ARG:HD3  | 2.28                     | 0.48              |
| 1:M:218:PRO:HB3  | 1:M:246:PRO:HG2  | 1.95                     | 0.48              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HB2  | 1.95                     | 0.48              |
| 1:N:361:ASP:HA   | 1:N:364:LYS:HE2  | 1.93                     | 0.48              |
| 2:P:73:VAL:HG13  | 2:P:86:MET:HB3   | 1.95                     | 0.48              |
| 1:F:350:ARG:HA   | 1:F:353:ILE:HD12 | 1.94                     | 0.48              |
| 1:I:361:ASP:O    | 1:I:365:LEU:HD23 | 2.13                     | 0.48              |
| 1:I:268:ARG:HG3  | 1:I:270:ILE:HG12 | 1.96                     | 0.48              |
| 1:F:226:LYS:NZ   | 1:F:227:ILE:O    | 2.46                     | 0.48              |
| 1:F:291:ASP:HB3  | 1:F:372:LEU:HD21 | 1.94                     | 0.48              |
| 1:J:218:PRO:HB3  | 1:J:246:PRO:HG2  | 1.96                     | 0.48              |
| 1:N:35:GLY:O     | 1:N:51:LYS:NZ    | 2.40                     | 0.48              |
| 2:P:40:VAL:HG23  | 2:P:62:GLY:H     | 1.78                     | 0.48              |
| 1:H:522:THR:OG1  | 1:I:41:ASP:OD2   | 2.29                     | 0.48              |
| 1:L:132:LYS:HZ3  | 1:L:501:ARG:HD3  | 1.78                     | 0.48              |
| 1:L:359:ASP:OD1  | 1:L:362:ARG:NH1  | 2.43                     | 0.48              |
| 1:A:197:ARG:HD2  | 1:A:277:LYS:HB2  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:40:LEU:HD22  | 1:B:59:GLU:HG2   | 1.95                     | 0.48              |
| 1:B:233:MET:HG3  | 1:B:237:LEU:HD13 | 1.95                     | 0.48              |
| 1:F:458:CYS:SG   | 1:F:480:ALA:HB1  | 2.54                     | 0.48              |
| 1:H:197:ARG:HE   | 1:H:279:PRO:HA   | 1.79                     | 0.48              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:HB2  | 1.95                     | 0.48              |
| 2:O:14:ARG:HH21  | 2:O:84:LEU:HD11  | 1.78                     | 0.48              |
| 1:F:325:ILE:HG12 | 1:F:330:THR:HG23 | 1.94                     | 0.48              |
| 1:K:87:ASP:OD1   | 1:K:88:GLY:N     | 2.46                     | 0.48              |
| 1:H:184:GLN:OE1  | 1:H:184:GLN:N    | 2.47                     | 0.47              |
| 1:N:361:ASP:HA   | 1:N:364:LYS:HZ1  | 1.79                     | 0.47              |
| 1:B:197:ARG:NH1  | 1:B:278:ALA:O    | 2.47                     | 0.47              |
| 1:G:360:TYR:O    | 1:G:364:LYS:HG2  | 2.14                     | 0.47              |
| 1:J:433:ASN:OD1  | 1:J:434:GLU:N    | 2.46                     | 0.47              |
| 1:E:349:ILE:HA   | 1:E:352:GLN:CD   | 2.39                     | 0.47              |
| 1:G:487:ASN:ND2  | 1:G:490:ASP:OD2  | 2.46                     | 0.47              |
| 1:J:69:MET:CE    | 1:J:522:THR:HB   | 2.44                     | 0.47              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:HB2  | 1.96                     | 0.47              |
| 2:T:73:VAL:HG12  | 2:T:84:LEU:HD12  | 1.95                     | 0.47              |
| 2:T:76:GLU:HG3   | 2:T:78:ILE:HG23  | 1.95                     | 0.47              |
| 1:A:458:CYS:SG   | 1:A:480:ALA:HB1  | 2.55                     | 0.47              |
| 1:H:122:LYS:HD3  | 1:H:440:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:226:LYS:HE2  | 1:B:253:ASP:HB3  | 1.96                     | 0.47              |
| 1:F:343:GLN:HA   | 1:F:346:VAL:HG22 | 1.96                     | 0.47              |
| 1:I:155:ASP:OD2  | 1:I:395:ARG:NH1  | 2.44                     | 0.47              |
| 1:C:219:PHE:CE1  | 1:C:245:LYS:HE2  | 2.50                     | 0.47              |
| 1:G:479:ASN:HB2  | 1:G:491:MET:HE1  | 1.96                     | 0.47              |
| 1:H:433:ASN:OD1  | 1:H:434:GLU:N    | 2.48                     | 0.47              |
| 1:I:383:ALA:HB3  | 1:I:389:MET:HB2  | 1.96                     | 0.47              |
| 1:J:18:ARG:NH1   | 1:J:67:GLU:OE2   | 2.45                     | 0.47              |
| 1:K:255:GLU:OE1  | 1:K:256:GLY:N    | 2.48                     | 0.47              |
| 1:B:228:SER:HA   | 1:B:255:GLU:HB2  | 1.96                     | 0.47              |
| 1:C:343:GLN:HA   | 1:C:346:VAL:HG22 | 1.96                     | 0.47              |
| 1:I:66:PHE:CD1   | 1:I:520:MET:HE3  | 2.49                     | 0.47              |
| 1:K:122:LYS:HD3  | 1:K:440:ILE:HD11 | 1.97                     | 0.47              |
| 1:C:23:LEU:HD22  | 1:C:74:VAL:HG13  | 1.97                     | 0.47              |
| 1:C:458:CYS:SG   | 1:C:480:ALA:HB1  | 2.54                     | 0.47              |
| 1:D:458:CYS:SG   | 1:D:480:ALA:HB1  | 2.55                     | 0.47              |
| 3:D:1600:ADP:O2A | 7:D:2001:HOH:O   | 2.20                     | 0.47              |
| 1:N:184:GLN:N    | 1:N:184:GLN:OE1  | 2.47                     | 0.47              |
| 2:U:67:PHE:CG    | 2:U:86:MET:HE1   | 2.50                     | 0.47              |
| 1:D:509:SER:OG   | 1:E:388:GLU:OE1  | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:GLU:HG3  | 1:E:380:LYS:HE2  | 1.97                     | 0.47              |
| 2:U:12:VAL:HG12  | 2:U:40:VAL:HG12  | 1.97                     | 0.47              |
| 1:A:284:ARG:O    | 1:A:288:MET:HG3  | 2.15                     | 0.46              |
| 1:F:267:MET:SD   | 1:F:268:ARG:HG2  | 2.55                     | 0.46              |
| 2:U:40:VAL:HG23  | 2:U:62:GLY:H     | 1.79                     | 0.46              |
| 1:B:487:ASN:O    | 1:B:491:MET:HG3  | 2.15                     | 0.46              |
| 1:F:487:ASN:ND2  | 1:F:490:ASP:OD2  | 2.48                     | 0.46              |
| 2:T:64:ILE:HB    | 2:T:95:VAL:HB    | 1.96                     | 0.46              |
| 1:A:219:PHE:HE2  | 1:A:245:LYS:HG3  | 1.80                     | 0.46              |
| 1:G:151:SER:HB2  | 1:G:399:ALA:HA   | 1.96                     | 0.46              |
| 1:H:361:ASP:HA   | 1:H:364:LYS:HE2  | 1.97                     | 0.46              |
| 1:I:69:MET:CE    | 1:I:522:THR:HB   | 2.45                     | 0.46              |
| 1:I:230:ILE:O    | 1:I:234:LEU:HG   | 2.16                     | 0.46              |
| 1:C:349:ILE:HG12 | 1:C:368:ARG:HH21 | 1.81                     | 0.46              |
| 1:J:69:MET:HE2   | 1:K:41:ASP:HB2   | 1.97                     | 0.46              |
| 1:L:284:ARG:O    | 1:L:288:MET:HG2  | 2.16                     | 0.46              |
| 1:M:66:PHE:CD1   | 1:M:520:MET:HE3  | 2.50                     | 0.46              |
| 1:A:349:ILE:HA   | 1:A:352:GLN:CD   | 2.40                     | 0.46              |
| 1:A:360:TYR:O    | 1:A:363:GLU:HG3  | 2.16                     | 0.46              |
| 1:H:127:ALA:HB2  | 1:H:447:MET:HE1  | 1.98                     | 0.46              |
| 1:M:188:ASP:N    | 1:M:188:ASP:OD1  | 2.48                     | 0.46              |
| 1:B:342:ILE:O    | 1:B:346:VAL:HG22 | 2.15                     | 0.46              |
| 1:I:188:ASP:OD1  | 1:I:188:ASP:N    | 2.47                     | 0.46              |
| 1:L:177:VAL:HG21 | 1:L:397:GLU:HG2  | 1.96                     | 0.46              |
| 1:L:188:ASP:OD1  | 1:L:188:ASP:N    | 2.49                     | 0.46              |
| 2:O:40:VAL:HG23  | 2:O:62:GLY:H     | 1.80                     | 0.46              |
| 1:A:305:ILE:HG21 | 1:A:307:MET:HE3  | 1.97                     | 0.46              |
| 1:A:511:ALA:O    | 1:A:515:ILE:HG12 | 2.15                     | 0.46              |
| 1:E:360:TYR:O    | 1:E:363:GLU:HG3  | 2.15                     | 0.46              |
| 1:F:5:ASP:HB2    | 1:F:524:LEU:HD23 | 1.98                     | 0.46              |
| 1:I:349:ILE:HG23 | 1:I:365:LEU:HD12 | 1.97                     | 0.46              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:HB2  | 1.97                     | 0.46              |
| 1:L:192:GLY:HA2  | 1:L:295:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:222:LEU:HD22 | 1:C:293:ALA:HB2  | 1.98                     | 0.46              |
| 1:C:487:ASN:O    | 1:C:491:MET:HG3  | 2.16                     | 0.46              |
| 1:D:69:MET:HE3   | 1:D:520:MET:HE2  | 1.98                     | 0.46              |
| 1:D:230:ILE:HG12 | 1:D:261:THR:HG21 | 1.97                     | 0.46              |
| 1:E:68:ASN:O     | 1:E:72:GLN:HG2   | 2.16                     | 0.46              |
| 1:C:291:ASP:HB3  | 1:C:372:LEU:HD11 | 1.97                     | 0.46              |
| 1:E:240:VAL:HG21 | 1:E:247:LEU:HD12 | 1.97                     | 0.46              |
| 1:I:525:PRO:C    | 1:I:526:LYS:HD2  | 2.41                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:188:ASP:OD1  | 1:J:188:ASP:N    | 2.48                     | 0.46              |
| 1:L:361:ASP:O    | 1:L:365:LEU:HD23 | 2.15                     | 0.46              |
| 1:M:284:ARG:O    | 1:M:288:MET:HG2  | 2.16                     | 0.46              |
| 1:E:260:ALA:O    | 1:E:264:VAL:HG23 | 2.15                     | 0.45              |
| 1:L:66:PHE:CD1   | 1:L:520:MET:HE3  | 2.52                     | 0.45              |
| 1:A:165:ALA:O    | 1:A:169:VAL:HG12 | 2.16                     | 0.45              |
| 1:H:218:PRO:HB3  | 1:H:246:PRO:HG2  | 1.98                     | 0.45              |
| 1:K:361:ASP:O    | 1:K:365:LEU:HD23 | 2.16                     | 0.45              |
| 1:A:259:LEU:O    | 1:A:263:VAL:HG22 | 2.17                     | 0.45              |
| 1:A:350:ARG:HA   | 1:A:353:ILE:HD12 | 1.98                     | 0.45              |
| 1:D:197:ARG:HE   | 1:D:279:PRO:HA   | 1.81                     | 0.45              |
| 1:G:510:VAL:O    | 1:G:514:MET:HG3  | 2.16                     | 0.45              |
| 1:K:66:PHE:CD1   | 1:K:520:MET:HE3  | 2.51                     | 0.45              |
| 1:L:388:GLU:HA   | 1:L:391:GLU:HG2  | 1.98                     | 0.45              |
| 1:D:479:ASN:HB2  | 1:D:491:MET:HE1  | 1.98                     | 0.45              |
| 1:M:284:ARG:HD3  | 1:M:364:LYS:HD2  | 1.98                     | 0.45              |
| 1:N:188:ASP:OD1  | 1:N:188:ASP:N    | 2.49                     | 0.45              |
| 1:A:68:ASN:O     | 1:A:72:GLN:HG2   | 2.17                     | 0.45              |
| 1:F:360:TYR:O    | 1:F:363:GLU:HG3  | 2.17                     | 0.45              |
| 1:M:230:ILE:HG22 | 1:M:233:MET:HE2  | 1.98                     | 0.45              |
| 1:M:362:ARG:O    | 1:M:366:GLN:HG2  | 2.16                     | 0.45              |
| 1:N:361:ASP:O    | 1:N:365:LEU:HD23 | 2.16                     | 0.45              |
| 1:C:68:ASN:O     | 1:C:72:GLN:HG2   | 2.16                     | 0.45              |
| 1:G:247:LEU:HD23 | 1:G:248:LEU:N    | 2.32                     | 0.45              |
| 1:H:188:ASP:N    | 1:H:188:ASP:OD1  | 2.48                     | 0.45              |
| 1:J:361:ASP:O    | 1:J:365:LEU:HD23 | 2.16                     | 0.45              |
| 1:D:124:VAL:HG21 | 1:D:508:ALA:CB   | 2.47                     | 0.45              |
| 1:N:224:ASP:HB3  | 1:N:302:SER:HB3  | 1.97                     | 0.45              |
| 1:A:220:ILE:HG23 | 1:A:250:ILE:HD12 | 1.98                     | 0.45              |
| 1:C:73:MET:HE2   | 1:C:73:MET:HA    | 1.98                     | 0.45              |
| 1:E:226:LYS:HD2  | 1:E:253:ASP:HB3  | 1.97                     | 0.45              |
| 1:F:68:ASN:O     | 1:F:72:GLN:HG2   | 2.17                     | 0.45              |
| 1:G:17:LEU:HD22  | 1:G:104:LEU:HD12 | 1.98                     | 0.45              |
| 1:G:281:PHE:H    | 1:G:284:ARG:HE   | 1.63                     | 0.45              |
| 1:A:365:LEU:O    | 1:A:369:VAL:HG23 | 2.17                     | 0.45              |
| 1:E:23:LEU:HD22  | 1:E:74:VAL:HG13  | 1.99                     | 0.45              |
| 1:H:177:VAL:HG11 | 1:H:397:GLU:HG2  | 1.99                     | 0.45              |
| 1:H:197:ARG:O    | 1:H:330:THR:OG1  | 2.29                     | 0.45              |
| 1:I:218:PRO:HB3  | 1:I:246:PRO:HG2  | 1.99                     | 0.45              |
| 1:C:360:TYR:O    | 1:C:363:GLU:HG3  | 2.17                     | 0.45              |
| 1:H:132:LYS:NZ   | 1:H:501:ARG:HD3  | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:601:ADP:O1B  | 7:I:701:HOH:O    | 2.21                     | 0.45              |
| 1:K:76:GLU:OE2   | 1:K:80:LYS:HE3   | 2.17                     | 0.45              |
| 1:B:458:CYS:SG   | 1:B:480:ALA:HB1  | 2.57                     | 0.44              |
| 1:G:458:CYS:SG   | 1:G:480:ALA:HB1  | 2.57                     | 0.44              |
| 1:B:169:VAL:HG12 | 1:B:173:GLY:HA3  | 2.00                     | 0.44              |
| 1:E:197:ARG:HD2  | 1:E:277:LYS:HB2  | 1.99                     | 0.44              |
| 1:E:266:THR:HG22 | 1:E:273:VAL:H    | 1.82                     | 0.44              |
| 1:H:66:PHE:CD1   | 1:H:520:MET:HE3  | 2.52                     | 0.44              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:HB2  | 1.99                     | 0.44              |
| 1:I:308:GLU:HB2  | 1:I:311:LYS:HG2  | 2.00                     | 0.44              |
| 1:K:197:ARG:HE   | 1:K:279:PRO:HA   | 1.81                     | 0.44              |
| 1:M:383:ALA:HB3  | 1:M:389:MET:HB2  | 1.99                     | 0.44              |
| 1:D:169:VAL:HG12 | 1:D:173:GLY:HA3  | 1.99                     | 0.44              |
| 1:E:247:LEU:HD23 | 1:E:248:LEU:N    | 2.32                     | 0.44              |
| 1:I:184:GLN:N    | 1:I:184:GLN:OE1  | 2.48                     | 0.44              |
| 1:J:367:GLU:HG2  | 1:J:371:LYS:HD3  | 1.98                     | 0.44              |
| 1:L:218:PRO:HB3  | 1:L:246:PRO:HG2  | 1.99                     | 0.44              |
| 1:M:197:ARG:HE   | 1:M:279:PRO:HA   | 1.83                     | 0.44              |
| 1:N:132:LYS:HZ1  | 1:N:501:ARG:HD3  | 1.81                     | 0.44              |
| 2:P:3:ILE:HD13   | 2:P:78:ILE:HG21  | 1.98                     | 0.44              |
| 2:Q:73:VAL:HG13  | 2:Q:86:MET:HB3   | 1.99                     | 0.44              |
| 2:S:57:LEU:HD22  | 2:S:88:GLU:HG3   | 1.98                     | 0.44              |
| 1:A:260:ALA:O    | 1:A:264:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:281:PHE:H    | 1:A:284:ARG:HE   | 1.66                     | 0.44              |
| 1:G:260:ALA:O    | 1:G:264:VAL:HG23 | 2.18                     | 0.44              |
| 2:O:73:VAL:HG12  | 2:O:84:LEU:HD12  | 1.99                     | 0.44              |
| 2:O:77:LYS:NZ    | 2:O:82:GLU:HB2   | 2.33                     | 0.44              |
| 2:T:40:VAL:HG23  | 2:T:62:GLY:H     | 1.83                     | 0.44              |
| 1:A:69:MET:HE2   | 1:A:522:THR:HB   | 1.98                     | 0.44              |
| 1:B:253:ASP:OD2  | 1:B:277:LYS:NZ   | 2.51                     | 0.44              |
| 1:B:360:TYR:O    | 1:B:363:GLU:HG3  | 2.17                     | 0.44              |
| 1:K:165:ALA:HB2  | 1:K:187:LEU:HD11 | 1.99                     | 0.44              |
| 1:L:291:ASP:OD2  | 1:L:368:ARG:NH1  | 2.50                     | 0.44              |
| 1:F:253:ASP:OD1  | 1:F:254:VAL:N    | 2.47                     | 0.44              |
| 1:K:349:ILE:HG23 | 1:K:365:LEU:HD12 | 1.99                     | 0.44              |
| 1:M:305:ILE:HB   | 1:M:307:MET:HE1  | 1.99                     | 0.44              |
| 1:C:230:ILE:HG12 | 1:C:261:THR:HG21 | 2.00                     | 0.44              |
| 1:D:68:ASN:O     | 1:D:72:GLN:HG2   | 2.17                     | 0.44              |
| 1:E:169:VAL:HG12 | 1:E:173:GLY:HA3  | 2.00                     | 0.44              |
| 1:K:224:ASP:HB3  | 1:K:302:SER:HB3  | 1.99                     | 0.44              |
| 1:N:353:ILE:HG12 | 1:N:365:LEU:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:U:46:GLY:HA2   | 2:U:57:LEU:HD22  | 2.00                     | 0.44              |
| 1:E:487:ASN:ND2  | 1:E:490:ASP:OD2  | 2.49                     | 0.44              |
| 1:H:224:ASP:HB3  | 1:H:302:SER:HB3  | 2.00                     | 0.44              |
| 1:I:419:LEU:HB3  | 1:I:447:MET:HB3  | 1.99                     | 0.44              |
| 1:L:61:GLU:O     | 1:L:62:LEU:HD23  | 2.18                     | 0.44              |
| 2:T:6:LEU:HB3    | 2:T:7:HIS:CD2    | 2.52                     | 0.44              |
| 2:T:68:ASN:HB3   | 2:U:74:LYS:HE2   | 1.98                     | 0.44              |
| 1:G:339:GLU:O    | 1:G:342:ILE:N    | 2.50                     | 0.44              |
| 1:G:343:GLN:HA   | 1:G:346:VAL:HG22 | 1.98                     | 0.44              |
| 1:H:353:ILE:HG12 | 1:H:365:LEU:HB3  | 2.00                     | 0.44              |
| 1:I:224:ASP:HB3  | 1:I:302:SER:HB3  | 2.00                     | 0.44              |
| 1:D:184:GLN:HA   | 1:D:184:GLN:OE1  | 2.18                     | 0.43              |
| 1:D:349:ILE:HA   | 1:D:352:GLN:CD   | 2.43                     | 0.43              |
| 1:F:169:VAL:HG12 | 1:F:173:GLY:HA3  | 2.00                     | 0.43              |
| 1:F:260:ALA:O    | 1:F:264:VAL:HG23 | 2.18                     | 0.43              |
| 1:M:263:VAL:HG12 | 1:M:267:MET:HE3  | 1.99                     | 0.43              |
| 1:B:68:ASN:O     | 1:B:72:GLN:HG2   | 2.19                     | 0.43              |
| 1:D:267:MET:SD   | 1:D:268:ARG:HG2  | 2.58                     | 0.43              |
| 1:E:17:LEU:HD22  | 1:E:104:LEU:HD12 | 2.00                     | 0.43              |
| 1:H:266:THR:HG22 | 1:H:273:VAL:H    | 1.82                     | 0.43              |
| 1:K:326:ASN:OD1  | 1:K:327:LYS:N    | 2.43                     | 0.43              |
| 1:K:345:ARG:O    | 1:K:349:ILE:HD12 | 2.17                     | 0.43              |
| 2:O:74:LYS:HE2   | 2:U:68:ASN:HB3   | 2.00                     | 0.43              |
| 2:Q:40:VAL:HG23  | 2:Q:62:GLY:H     | 1.83                     | 0.43              |
| 2:R:77:LYS:NZ    | 2:R:82:GLU:HB2   | 2.34                     | 0.43              |
| 1:A:345:ARG:O    | 1:A:349:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:348:GLN:O    | 1:A:352:GLN:OE1  | 2.35                     | 0.43              |
| 1:B:219:PHE:HB3  | 1:B:317:LEU:HD23 | 2.00                     | 0.43              |
| 1:E:509:SER:OG   | 1:F:388:GLU:OE1  | 2.29                     | 0.43              |
| 1:F:360:TYR:O    | 1:F:364:LYS:HG2  | 2.18                     | 0.43              |
| 1:G:68:ASN:O     | 1:G:72:GLN:HG2   | 2.18                     | 0.43              |
| 1:I:388:GLU:HA   | 1:I:391:GLU:HG3  | 2.00                     | 0.43              |
| 3:J:601:ADP:O1B  | 7:J:802:HOH:O    | 2.21                     | 0.43              |
| 1:C:165:ALA:O    | 1:C:169:VAL:HG12 | 2.19                     | 0.43              |
| 1:H:76:GLU:OE2   | 1:H:80:LYS:HE3   | 2.18                     | 0.43              |
| 1:J:196:ASP:N    | 1:J:196:ASP:OD1  | 2.45                     | 0.43              |
| 2:S:77:LYS:NZ    | 2:S:80:ASN:HA    | 2.32                     | 0.43              |
| 1:F:193:MET:SD   | 1:F:292:ILE:HG12 | 2.59                     | 0.43              |
| 1:G:169:VAL:HG12 | 1:G:173:GLY:HA3  | 2.00                     | 0.43              |
| 1:G:349:ILE:HA   | 1:G:352:GLN:CD   | 2.43                     | 0.43              |
| 1:G:429:LEU:C    | 1:G:430:ARG:HD2  | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:158:VAL:HG13 | 1:M:396:VAL:HG22 | 2.01                     | 0.43              |
| 1:N:177:VAL:HG21 | 1:N:397:GLU:HG2  | 1.99                     | 0.43              |
| 1:C:305:ILE:HG21 | 1:C:307:MET:HE3  | 2.01                     | 0.43              |
| 1:G:217:SER:N    | 1:G:218:PRO:HD3  | 2.33                     | 0.43              |
| 1:H:284:ARG:HG2  | 1:H:288:MET:HE2  | 2.01                     | 0.43              |
| 1:K:161:LEU:HD11 | 1:K:185:ASP:HB3  | 2.00                     | 0.43              |
| 1:K:188:ASP:N    | 1:K:188:ASP:OD1  | 2.49                     | 0.43              |
| 1:M:522:THR:OG1  | 1:N:41:ASP:OD2   | 2.35                     | 0.43              |
| 1:A:222:LEU:HD23 | 1:A:250:ILE:HB   | 2.01                     | 0.43              |
| 1:C:194:GLN:HG3  | 1:C:331:THR:HB   | 2.00                     | 0.43              |
| 1:E:458:CYS:SG   | 1:E:480:ALA:HB1  | 2.58                     | 0.43              |
| 1:J:132:LYS:HZ1  | 1:J:501:ARG:HD3  | 1.84                     | 0.43              |
| 1:M:361:ASP:O    | 1:M:365:LEU:HD23 | 2.19                     | 0.43              |
| 2:U:64:ILE:HB    | 2:U:95:VAL:HB    | 2.01                     | 0.43              |
| 1:C:347:ALA:O    | 1:C:351:GLN:HG3  | 2.19                     | 0.43              |
| 1:D:187:LEU:HD11 | 1:D:377:ALA:HB1  | 2.01                     | 0.43              |
| 1:G:266:THR:HG22 | 1:G:273:VAL:H    | 1.84                     | 0.43              |
| 1:H:362:ARG:O    | 1:H:366:GLN:HG2  | 2.19                     | 0.43              |
| 1:D:348:GLN:O    | 1:D:352:GLN:OE1  | 2.37                     | 0.43              |
| 1:E:511:ALA:O    | 1:E:515:ILE:HG12 | 2.18                     | 0.43              |
| 1:H:198:GLY:O    | 1:H:276:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:193:MET:SD   | 1:A:292:ILE:HG12 | 2.58                     | 0.42              |
| 1:H:345:ARG:O    | 1:H:349:ILE:HD12 | 2.19                     | 0.42              |
| 1:A:69:MET:O     | 1:A:73:MET:HG3   | 2.19                     | 0.42              |
| 1:D:260:ALA:O    | 1:D:264:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:347:ALA:O    | 1:D:350:ARG:HG2  | 2.20                     | 0.42              |
| 1:E:348:GLN:O    | 1:E:352:GLN:OE1  | 2.38                     | 0.42              |
| 1:I:295:LEU:HA   | 1:I:342:ILE:HD11 | 2.02                     | 0.42              |
| 2:Q:76:GLU:HG3   | 2:Q:78:ILE:HG23  | 2.01                     | 0.42              |
| 2:T:67:PHE:CG    | 2:T:86:MET:HE1   | 2.54                     | 0.42              |
| 1:B:144:ILE:HG23 | 1:B:403:THR:CG2  | 2.50                     | 0.42              |
| 1:J:155:ASP:OD2  | 1:J:395:ARG:NH1  | 2.52                     | 0.42              |
| 1:L:383:ALA:HB3  | 1:L:389:MET:HB2  | 2.01                     | 0.42              |
| 1:M:250:ILE:HD11 | 1:M:278:ALA:HA   | 2.01                     | 0.42              |
| 1:B:239:ALA:HB1  | 1:B:314:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:230:ILE:HD12 | 1:C:233:MET:HE3  | 2.02                     | 0.42              |
| 1:C:348:GLN:O    | 1:C:352:GLN:OE1  | 2.37                     | 0.42              |
| 1:J:184:GLN:OE1  | 1:J:184:GLN:N    | 2.50                     | 0.42              |
| 1:M:177:VAL:HG21 | 1:M:397:GLU:HG2  | 2.00                     | 0.42              |
| 1:B:350:ARG:HA   | 1:B:353:ILE:HD12 | 2.01                     | 0.42              |
| 1:G:87:ASP:OD2   | 1:G:88:GLY:N     | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:511:ALA:O    | 1:G:515:ILE:HG12 | 2.20                     | 0.42              |
| 1:H:361:ASP:O    | 1:H:365:LEU:HD23 | 2.19                     | 0.42              |
| 2:R:78:ILE:O     | 2:R:81:GLU:N     | 2.50                     | 0.42              |
| 2:T:6:LEU:HB3    | 2:T:7:HIS:HD2    | 1.85                     | 0.42              |
| 1:C:124:VAL:HG21 | 1:C:508:ALA:CB   | 2.50                     | 0.42              |
| 1:D:124:VAL:HG21 | 1:D:508:ALA:HB2  | 2.02                     | 0.42              |
| 1:G:347:ALA:O    | 1:G:351:GLN:OE1  | 2.38                     | 0.42              |
| 1:H:361:ASP:HA   | 1:H:364:LYS:HZ1  | 1.85                     | 0.42              |
| 1:H:473:ASP:N    | 1:H:473:ASP:OD1  | 2.53                     | 0.42              |
| 1:J:158:VAL:HG13 | 1:J:396:VAL:HG22 | 2.01                     | 0.42              |
| 1:D:221:LEU:HD23 | 1:D:249:ILE:HG12 | 2.02                     | 0.42              |
| 1:F:348:GLN:O    | 1:F:352:GLN:OE1  | 2.38                     | 0.42              |
| 1:H:367:GLU:HG2  | 1:H:371:LYS:HE2  | 2.02                     | 0.42              |
| 1:J:61:GLU:O     | 1:J:62:LEU:HD23  | 2.20                     | 0.42              |
| 1:J:345:ARG:O    | 1:J:349:ILE:HD12 | 2.19                     | 0.42              |
| 1:K:301:ILE:HG21 | 1:K:309:LEU:HD23 | 2.01                     | 0.42              |
| 1:L:345:ARG:O    | 1:L:349:ILE:HD12 | 2.19                     | 0.42              |
| 1:N:473:ASP:OD1  | 1:N:473:ASP:N    | 2.53                     | 0.42              |
| 2:O:6:LEU:HB3    | 2:O:7:HIS:CD2    | 2.55                     | 0.42              |
| 1:A:488:MET:HA   | 1:A:488:MET:HE2  | 2.02                     | 0.42              |
| 1:B:291:ASP:HB3  | 1:B:372:LEU:HD11 | 2.00                     | 0.42              |
| 1:C:205:ILE:HA   | 1:C:213:VAL:HG22 | 2.00                     | 0.42              |
| 1:G:360:TYR:O    | 1:G:363:GLU:HG3  | 2.19                     | 0.42              |
| 1:L:158:VAL:HG13 | 1:L:396:VAL:HG22 | 2.02                     | 0.42              |
| 1:M:76:GLU:OE2   | 1:M:80:LYS:NZ    | 2.47                     | 0.42              |
| 2:O:64:ILE:HB    | 2:O:95:VAL:HB    | 2.02                     | 0.42              |
| 1:B:222:LEU:HD23 | 1:B:250:ILE:HB   | 2.02                     | 0.42              |
| 1:C:226:LYS:NZ   | 1:C:255:GLU:HG2  | 2.35                     | 0.42              |
| 1:E:193:MET:SD   | 1:E:292:ILE:HG12 | 2.60                     | 0.42              |
| 1:F:226:LYS:HE2  | 1:F:253:ASP:HB3  | 2.01                     | 0.42              |
| 1:G:348:GLN:O    | 1:G:352:GLN:OE1  | 2.37                     | 0.42              |
| 2:P:74:LYS:HE3   | 2:P:74:LYS:HB3   | 1.77                     | 0.42              |
| 1:A:348:GLN:HA   | 1:A:351:GLN:OE1  | 2.20                     | 0.42              |
| 1:B:169:VAL:HG21 | 1:B:377:ALA:HB2  | 2.02                     | 0.42              |
| 1:B:349:ILE:HA   | 1:B:352:GLN:CD   | 2.45                     | 0.42              |
| 1:E:233:MET:HG2  | 1:E:309:LEU:HD21 | 2.01                     | 0.42              |
| 1:G:239:ALA:HB1  | 1:G:314:LEU:HD21 | 2.01                     | 0.42              |
| 1:I:35:GLY:O     | 1:I:51:LYS:NZ    | 2.40                     | 0.42              |
| 1:L:473:ASP:N    | 1:L:473:ASP:OD1  | 2.53                     | 0.42              |
| 3:L:601:ADP:O1B  | 7:L:802:HOH:O    | 2.21                     | 0.42              |
| 1:N:255:GLU:OE2  | 1:N:257:GLU:HG2  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:48:THR:HG22  | 1:H:50:THR:HG23  | 2.00                     | 0.41              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:HB2  | 2.02                     | 0.41              |
| 1:F:125:THR:O    | 1:F:129:GLU:OE1  | 2.38                     | 0.41              |
| 1:G:260:ALA:HA   | 1:G:263:VAL:HG12 | 2.02                     | 0.41              |
| 1:I:488:MET:HE3  | 1:I:493:ILE:HB   | 2.01                     | 0.41              |
| 1:K:52:ASP:O     | 1:K:56:VAL:HG23  | 2.20                     | 0.41              |
| 1:M:217:SER:HA   | 1:M:320:ALA:O    | 2.20                     | 0.41              |
| 2:R:12:VAL:HG12  | 2:R:40:VAL:HG12  | 2.01                     | 0.41              |
| 1:D:226:LYS:NZ   | 1:D:227:ILE:O    | 2.53                     | 0.41              |
| 1:G:169:VAL:CG1  | 1:G:173:GLY:HA3  | 2.50                     | 0.41              |
| 1:H:61:GLU:O     | 1:H:62:LEU:HD23  | 2.19                     | 0.41              |
| 1:H:200:LEU:HD12 | 1:H:275:ALA:HB1  | 2.01                     | 0.41              |
| 1:L:250:ILE:HD11 | 1:L:278:ALA:HA   | 2.01                     | 0.41              |
| 3:C:1600:ADP:O1B | 5:C:1602:BEF:F1  | 2.26                     | 0.41              |
| 1:E:69:MET:CE    | 1:E:522:THR:HB   | 2.46                     | 0.41              |
| 1:E:287:ALA:HB1  | 1:E:368:ARG:NH2  | 2.35                     | 0.41              |
| 1:G:184:GLN:HA   | 1:G:184:GLN:OE1  | 2.21                     | 0.41              |
| 1:G:226:LYS:NZ   | 1:G:255:GLU:HG2  | 2.35                     | 0.41              |
| 1:G:339:GLU:HA   | 1:G:342:ILE:HD13 | 2.03                     | 0.41              |
| 1:H:441:LYS:HD3  | 1:H:441:LYS:HA   | 1.84                     | 0.41              |
| 1:L:52:ASP:O     | 1:L:56:VAL:HG23  | 2.20                     | 0.41              |
| 1:L:217:SER:HA   | 1:L:320:ALA:O    | 2.21                     | 0.41              |
| 1:N:358:SER:HB3  | 1:N:361:ASP:HB2  | 2.03                     | 0.41              |
| 2:S:67:PHE:CG    | 2:S:86:MET:HE1   | 2.55                     | 0.41              |
| 1:A:349:ILE:HA   | 1:A:352:GLN:NE2  | 2.36                     | 0.41              |
| 1:L:301:ILE:HG21 | 1:L:309:LEU:HD23 | 2.01                     | 0.41              |
| 1:N:217:SER:HA   | 1:N:320:ALA:O    | 2.20                     | 0.41              |
| 1:A:124:VAL:HG21 | 1:A:508:ALA:CB   | 2.50                     | 0.41              |
| 1:A:287:ALA:HB1  | 1:A:368:ARG:NH2  | 2.36                     | 0.41              |
| 1:G:23:LEU:HD22  | 1:G:74:VAL:HG13  | 2.03                     | 0.41              |
| 3:K:601:ADP:O1B  | 7:K:701:HOH:O    | 2.22                     | 0.41              |
| 1:L:419:LEU:HB3  | 1:L:447:MET:HB3  | 2.01                     | 0.41              |
| 1:N:66:PHE:CD1   | 1:N:520:MET:HE3  | 2.52                     | 0.41              |
| 1:N:200:LEU:HD12 | 1:N:275:ALA:HB1  | 2.02                     | 0.41              |
| 2:O:11:ILE:HB    | 2:O:42:ALA:HB3   | 2.01                     | 0.41              |
| 1:I:473:ASP:OD1  | 1:I:473:ASP:N    | 2.53                     | 0.41              |
| 1:B:348:GLN:O    | 1:B:352:GLN:OE1  | 2.38                     | 0.41              |
| 1:E:124:VAL:HG21 | 1:E:508:ALA:CB   | 2.51                     | 0.41              |
| 1:E:347:ALA:O    | 1:E:351:GLN:OE1  | 2.39                     | 0.41              |
| 1:F:169:VAL:CG1  | 1:F:173:GLY:HA3  | 2.50                     | 0.41              |
| 1:G:220:ILE:HG23 | 1:G:250:ILE:HD12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:289:LEU:HD23 | 1:G:289:LEU:HA   | 1.92                     | 0.41              |
| 1:L:353:ILE:HG12 | 1:L:365:LEU:HB3  | 2.02                     | 0.41              |
| 2:T:37:ARG:HH22  | 2:U:78:ILE:HG22  | 1.85                     | 0.41              |
| 1:A:239:ALA:HB1  | 1:A:314:LEU:HD11 | 2.03                     | 0.41              |
| 1:D:220:ILE:HG23 | 1:D:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:E:325:ILE:HG12 | 1:E:330:THR:HG23 | 2.03                     | 0.41              |
| 1:G:124:VAL:HG21 | 1:G:508:ALA:CB   | 2.51                     | 0.41              |
| 1:H:421:ARG:HD3  | 1:H:421:ARG:HA   | 1.93                     | 0.41              |
| 1:I:158:VAL:HG13 | 1:I:396:VAL:HG22 | 2.03                     | 0.41              |
| 1:J:197:ARG:O    | 1:J:330:THR:OG1  | 2.30                     | 0.41              |
| 1:K:158:VAL:HG13 | 1:K:396:VAL:HG22 | 2.03                     | 0.41              |
| 1:K:434:GLU:O    | 1:K:438:VAL:HG23 | 2.20                     | 0.41              |
| 1:L:17:LEU:HD12  | 1:L:17:LEU:HA    | 1.90                     | 0.41              |
| 1:L:197:ARG:HE   | 1:L:279:PRO:HA   | 1.86                     | 0.41              |
| 1:L:487:ASN:O    | 1:L:491:MET:HG3  | 2.20                     | 0.41              |
| 2:O:46:GLY:HA2   | 2:O:57:LEU:HD22  | 2.02                     | 0.41              |
| 2:Q:73:VAL:HG11  | 2:Q:84:LEU:HD23  | 2.03                     | 0.41              |
| 2:S:78:ILE:HD11  | 2:S:83:VAL:HG11  | 2.03                     | 0.41              |
| 1:B:266:THR:HG22 | 1:B:273:VAL:H    | 1.85                     | 0.41              |
| 1:D:106:ALA:O    | 1:D:111:MET:HE2  | 2.21                     | 0.41              |
| 1:D:228:SER:HA   | 1:D:255:GLU:HB2  | 2.03                     | 0.41              |
| 1:J:224:ASP:HB3  | 1:J:302:SER:HB3  | 2.03                     | 0.41              |
| 2:S:4:ARG:HA     | 2:S:5:PRO:HD3    | 1.95                     | 0.41              |
| 1:D:347:ALA:O    | 1:D:351:GLN:OE1  | 2.39                     | 0.40              |
| 1:L:266:THR:HG22 | 1:L:273:VAL:H    | 1.86                     | 0.40              |
| 1:D:278:ALA:HB3  | 1:D:285:ARG:HD2  | 2.04                     | 0.40              |
| 1:F:347:ALA:O    | 1:F:351:GLN:OE1  | 2.39                     | 0.40              |
| 1:I:345:ARG:O    | 1:I:349:ILE:HD12 | 2.21                     | 0.40              |
| 1:K:200:LEU:HD12 | 1:K:275:ALA:HB1  | 2.02                     | 0.40              |
| 1:K:283:ASP:O    | 1:K:286:LYS:HG3  | 2.21                     | 0.40              |
| 1:L:326:ASN:OD1  | 1:L:327:LYS:N    | 2.42                     | 0.40              |
| 1:A:150:ILE:HD13 | 1:A:150:ILE:HA   | 1.94                     | 0.40              |
| 1:C:73:MET:HE3   | 1:D:47:PRO:HD2   | 2.03                     | 0.40              |
| 1:D:291:ASP:OD1  | 1:D:345:ARG:NE   | 2.44                     | 0.40              |
| 1:G:364:LYS:HA   | 1:G:364:LYS:HD2  | 1.94                     | 0.40              |
| 1:G:389:MET:HE2  | 1:G:389:MET:HB2  | 1.99                     | 0.40              |
| 1:K:18:ARG:NH2   | 1:K:67:GLU:OE2   | 2.45                     | 0.40              |
| 1:L:270:ILE:HG22 | 1:L:271:VAL:HG23 | 2.03                     | 0.40              |
| 2:O:78:ILE:O     | 2:O:81:GLU:N     | 2.52                     | 0.40              |
| 2:S:73:VAL:HG12  | 2:S:84:LEU:HD12  | 2.03                     | 0.40              |
| 1:B:237:LEU:HA   | 1:B:240:VAL:HG22 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:262:LEU:O    | 1:D:266:THR:HG23 | 2.22                     | 0.40              |
| 1:K:177:VAL:HG21 | 1:K:397:GLU:HG2  | 2.03                     | 0.40              |
| 1:N:345:ARG:O    | 1:N:349:ILE:HD12 | 2.20                     | 0.40              |
| 1:A:226:LYS:NZ   | 1:A:227:ILE:O    | 2.55                     | 0.40              |
| 1:E:125:THR:O    | 1:E:129:GLU:HG2  | 2.21                     | 0.40              |
| 1:K:197:ARG:O    | 1:K:330:THR:OG1  | 2.29                     | 0.40              |
| 1:K:473:ASP:OD1  | 1:K:473:ASP:N    | 2.52                     | 0.40              |
| 1:M:473:ASP:N    | 1:M:473:ASP:OD1  | 2.53                     | 0.40              |
| 2:Q:8:ASP:HA     | 2:Q:57:LEU:HD11  | 2.04                     | 0.40              |
| 2:T:12:VAL:HG12  | 2:T:40:VAL:HG12  | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 522/547 (95%) | 511 (98%) | 11 (2%) | 0        | 100         | 100 |
| 1   | B     | 522/547 (95%) | 514 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | C     | 522/547 (95%) | 516 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 1   | D     | 522/547 (95%) | 515 (99%) | 7 (1%)  | 0        | 100         | 100 |
| 1   | E     | 522/547 (95%) | 514 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | F     | 522/547 (95%) | 515 (99%) | 7 (1%)  | 0        | 100         | 100 |
| 1   | G     | 522/547 (95%) | 514 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | H     | 523/547 (96%) | 514 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | I     | 523/547 (96%) | 513 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | J     | 523/547 (96%) | 511 (98%) | 12 (2%) | 0        | 100         | 100 |
| 1   | K     | 523/547 (96%) | 512 (98%) | 11 (2%) | 0        | 100         | 100 |
| 1   | L     | 523/547 (96%) | 511 (98%) | 12 (2%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | M     | 523/547 (96%)   | 516 (99%)  | 7 (1%)   | 0        | 100         | 100 |
| 1   | N     | 523/547 (96%)   | 514 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 2   | O     | 93/97 (96%)     | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | P     | 93/97 (96%)     | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | Q     | 93/97 (96%)     | 92 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 2   | R     | 93/97 (96%)     | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | S     | 93/97 (96%)     | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | T     | 93/97 (96%)     | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | U     | 93/97 (96%)     | 92 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| All | All   | 7966/8337 (96%) | 7829 (98%) | 137 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | B     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | C     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | D     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | E     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | F     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | G     | 403/414 (97%) | 403 (100%) | 0        | 100         | 100 |
| 1   | H     | 405/414 (98%) | 405 (100%) | 0        | 100         | 100 |
| 1   | I     | 405/414 (98%) | 405 (100%) | 0        | 100         | 100 |
| 1   | J     | 405/414 (98%) | 405 (100%) | 0        | 100         | 100 |
| 1   | K     | 405/414 (98%) | 405 (100%) | 0        | 100         | 100 |
| 1   | L     | 405/414 (98%) | 405 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | M     | 405/414 (98%)   | 405 (100%)  | 0        | 100         | 100 |
| 1   | N     | 405/414 (98%)   | 405 (100%)  | 0        | 100         | 100 |
| 2   | O     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | P     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | Q     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | R     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | S     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | T     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| 2   | U     | 73/80 (91%)     | 73 (100%)   | 0        | 100         | 100 |
| All | All   | 6167/6356 (97%) | 6167 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 290 | GLN  |
| 1   | B     | 37  | ASN  |
| 1   | B     | 184 | GLN  |
| 1   | B     | 433 | ASN  |
| 1   | C     | 290 | GLN  |
| 1   | C     | 343 | GLN  |
| 1   | C     | 453 | GLN  |
| 1   | E     | 290 | GLN  |
| 1   | F     | 343 | GLN  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 433 | ASN  |
| 1   | H     | 37  | ASN  |
| 1   | H     | 68  | ASN  |
| 1   | H     | 72  | GLN  |
| 1   | H     | 82  | ASN  |
| 1   | H     | 290 | GLN  |
| 1   | H     | 401 | HIS  |
| 1   | H     | 453 | GLN  |
| 1   | I     | 68  | ASN  |
| 1   | I     | 72  | GLN  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 229 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 290 | GLN  |
| 1   | I     | 401 | HIS  |
| 1   | I     | 453 | GLN  |
| 1   | I     | 487 | ASN  |
| 1   | J     | 37  | ASN  |
| 1   | J     | 68  | ASN  |
| 1   | J     | 72  | GLN  |
| 1   | J     | 112 | ASN  |
| 1   | J     | 146 | GLN  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 401 | HIS  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 475 | ASN  |
| 1   | K     | 68  | ASN  |
| 1   | K     | 72  | GLN  |
| 1   | K     | 82  | ASN  |
| 1   | L     | 68  | ASN  |
| 1   | L     | 72  | GLN  |
| 1   | L     | 82  | ASN  |
| 1   | L     | 112 | ASN  |
| 1   | L     | 290 | GLN  |
| 1   | L     | 401 | HIS  |
| 1   | L     | 453 | GLN  |
| 1   | L     | 487 | ASN  |
| 1   | M     | 37  | ASN  |
| 1   | M     | 68  | ASN  |
| 1   | M     | 72  | GLN  |
| 1   | M     | 82  | ASN  |
| 1   | M     | 290 | GLN  |
| 1   | M     | 453 | GLN  |
| 1   | N     | 68  | ASN  |
| 1   | N     | 72  | GLN  |
| 1   | N     | 82  | ASN  |
| 1   | N     | 112 | ASN  |
| 1   | N     | 401 | HIS  |
| 1   | N     | 453 | GLN  |
| 1   | N     | 487 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 28 are monoatomic - leaving 21 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | ADP  | J     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.96 | 10 (23%)    |
| 3   | ADP  | I     | 601  | 4,6   | 27,29,29     | 1.34 | 5 (18%)     | 42,45,45    | 1.94 | 10 (23%)    |
| 3   | ADP  | K     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.93 | 10 (23%)    |
| 5   | BEF  | C     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 3   | ADP  | F     | 1600 | 4,5,6 | 27,29,29     | 1.33 | 5 (18%)     | 42,45,45    | 1.92 | 10 (23%)    |
| 3   | ADP  | L     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.91 | 10 (23%)    |
| 3   | ADP  | B     | 1600 | 4,5,6 | 27,29,29     | 1.34 | 5 (18%)     | 42,45,45    | 1.90 | 11 (26%)    |
| 3   | ADP  | C     | 1600 | 4,5,6 | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.91 | 10 (23%)    |
| 5   | BEF  | F     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 3   | ADP  | G     | 1600 | 4,5,6 | 27,29,29     | 1.33 | 5 (18%)     | 42,45,45    | 1.91 | 10 (23%)    |
| 3   | ADP  | H     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.94 | 9 (21%)     |
| 3   | ADP  | M     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.93 | 10 (23%)    |
| 3   | ADP  | D     | 1600 | 4,5,6 | 27,29,29     | 1.34 | 5 (18%)     | 42,45,45    | 1.92 | 9 (21%)     |
| 5   | BEF  | D     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 5   | BEF  | G     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 5   | BEF  | B     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 5   | BEF  | E     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |
| 3   | ADP  | N     | 601  | 4,6   | 27,29,29     | 1.34 | 4 (14%)     | 42,45,45    | 1.94 | 10 (23%)    |
| 5   | BEF  | A     | 1602 | 3     | 0,3,3        | -    | -           | -           | -    | -           |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ADP  | E     | 1600 | 4,5,6 | 27,29,29     | 1.34 | 4 (14%)  | 42,45,45    | 1.91 | 10 (23%) |
| 3   | ADP  | A     | 1600 | 4,5,6 | 27,29,29     | 1.33 | 5 (18%)  | 42,45,45    | 1.90 | 10 (23%) |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions    | Rings   |
|-----|------|-------|------|-------|---------|-------------|---------|
| 3   | ADP  | J     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | F     | 1600 | 4,5,6 | -       | 10/16/32/32 | 0/3/3/3 |
| 3   | ADP  | N     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | D     | 1600 | 4,5,6 | -       | 6/16/32/32  | 0/3/3/3 |
| 3   | ADP  | L     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | I     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | K     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | E     | 1600 | 4,5,6 | -       | 8/16/32/32  | 0/3/3/3 |
| 3   | ADP  | G     | 1600 | 4,5,6 | -       | 8/16/32/32  | 0/3/3/3 |
| 3   | ADP  | B     | 1600 | 4,5,6 | -       | 8/16/32/32  | 0/3/3/3 |
| 3   | ADP  | C     | 1600 | 4,5,6 | -       | 10/16/32/32 | 0/3/3/3 |
| 3   | ADP  | A     | 1600 | 4,5,6 | -       | 8/16/32/32  | 0/3/3/3 |
| 3   | ADP  | H     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |
| 3   | ADP  | M     | 601  | 4,6   | -       | 7/16/32/32  | 0/3/3/3 |

All (62) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | H     | 601  | ADP  | C5-C4 | 4.26 | 1.47        | 1.39     |
| 3   | I     | 601  | ADP  | C5-C4 | 4.24 | 1.46        | 1.39     |
| 3   | J     | 601  | ADP  | C5-C4 | 4.23 | 1.46        | 1.39     |
| 3   | N     | 601  | ADP  | C5-C4 | 4.23 | 1.46        | 1.39     |
| 3   | M     | 601  | ADP  | C5-C4 | 4.21 | 1.46        | 1.39     |
| 3   | K     | 601  | ADP  | C5-C4 | 4.19 | 1.46        | 1.39     |
| 3   | L     | 601  | ADP  | C5-C4 | 4.17 | 1.46        | 1.39     |
| 3   | C     | 1600 | ADP  | C5-C4 | 4.15 | 1.46        | 1.39     |
| 3   | E     | 1600 | ADP  | C5-C4 | 4.11 | 1.46        | 1.39     |
| 3   | D     | 1600 | ADP  | C5-C4 | 4.09 | 1.46        | 1.39     |
| 3   | G     | 1600 | ADP  | C5-C4 | 4.05 | 1.46        | 1.39     |
| 3   | A     | 1600 | ADP  | C5-C4 | 4.01 | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | F     | 1600 | ADP  | C5-C4 | 4.01  | 1.46        | 1.39     |
| 3   | B     | 1600 | ADP  | C5-C4 | 4.01  | 1.46        | 1.39     |
| 3   | B     | 1600 | ADP  | C5-C6 | 2.58  | 1.48        | 1.41     |
| 3   | L     | 601  | ADP  | C5-C6 | 2.56  | 1.48        | 1.41     |
| 3   | M     | 601  | ADP  | C5-C6 | 2.55  | 1.48        | 1.41     |
| 3   | E     | 1600 | ADP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 3   | C     | 1600 | ADP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 3   | H     | 601  | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | N     | 601  | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | G     | 1600 | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | K     | 601  | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | D     | 1600 | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 3   | I     | 601  | ADP  | C5-C6 | 2.52  | 1.48        | 1.41     |
| 3   | J     | 601  | ADP  | C5-C6 | 2.50  | 1.48        | 1.41     |
| 3   | A     | 1600 | ADP  | C5-C6 | 2.48  | 1.48        | 1.41     |
| 3   | F     | 1600 | ADP  | C5-C6 | 2.48  | 1.48        | 1.41     |
| 3   | E     | 1600 | ADP  | C5-N7 | -2.39 | 1.34        | 1.39     |
| 3   | F     | 1600 | ADP  | C5-N7 | -2.36 | 1.34        | 1.39     |
| 3   | C     | 1600 | ADP  | C5-N7 | -2.36 | 1.34        | 1.39     |
| 3   | B     | 1600 | ADP  | C5-N7 | -2.35 | 1.34        | 1.39     |
| 3   | H     | 601  | ADP  | C5-N7 | -2.34 | 1.34        | 1.39     |
| 3   | G     | 1600 | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 3   | M     | 601  | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 3   | D     | 1600 | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 3   | A     | 1600 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 3   | J     | 601  | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 3   | L     | 601  | ADP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 3   | K     | 601  | ADP  | C8-N7 | 2.26  | 1.35        | 1.31     |
| 3   | N     | 601  | ADP  | C5-N7 | -2.26 | 1.34        | 1.39     |
| 3   | K     | 601  | ADP  | C5-N7 | -2.25 | 1.34        | 1.39     |
| 3   | I     | 601  | ADP  | C5-N7 | -2.25 | 1.34        | 1.39     |
| 3   | L     | 601  | ADP  | C8-N7 | 2.24  | 1.35        | 1.31     |
| 3   | M     | 601  | ADP  | C8-N7 | 2.22  | 1.35        | 1.31     |
| 3   | D     | 1600 | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 3   | G     | 1600 | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 3   | N     | 601  | ADP  | C8-N7 | 2.20  | 1.35        | 1.31     |
| 3   | I     | 601  | ADP  | C8-N7 | 2.18  | 1.35        | 1.31     |
| 3   | J     | 601  | ADP  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 3   | H     | 601  | ADP  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 3   | F     | 1600 | ADP  | C8-N7 | 2.15  | 1.35        | 1.31     |
| 3   | B     | 1600 | ADP  | C8-N7 | 2.13  | 1.35        | 1.31     |
| 3   | E     | 1600 | ADP  | C8-N7 | 2.13  | 1.35        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | A     | 1600 | ADP  | C8-N7 | 2.11  | 1.35        | 1.31     |
| 3   | B     | 1600 | ADP  | C4-N9 | -2.10 | 1.33        | 1.37     |
| 3   | A     | 1600 | ADP  | C4-N9 | -2.09 | 1.33        | 1.37     |
| 3   | C     | 1600 | ADP  | C8-N7 | 2.08  | 1.35        | 1.31     |
| 3   | D     | 1600 | ADP  | C4-N9 | -2.06 | 1.33        | 1.37     |
| 3   | F     | 1600 | ADP  | C4-N9 | -2.06 | 1.33        | 1.37     |
| 3   | G     | 1600 | ADP  | C4-N9 | -2.06 | 1.33        | 1.37     |
| 3   | I     | 601  | ADP  | C4-N9 | -2.01 | 1.33        | 1.37     |

All (139) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | J     | 601  | ADP  | C5-C4-N3 | -6.17 | 118.69      | 126.75   |
| 3   | H     | 601  | ADP  | C5-C4-N3 | -6.14 | 118.75      | 126.75   |
| 3   | E     | 1600 | ADP  | C5-C4-N3 | -6.12 | 118.77      | 126.75   |
| 3   | N     | 601  | ADP  | C5-C4-N3 | -6.11 | 118.78      | 126.75   |
| 3   | I     | 601  | ADP  | C5-C4-N3 | -6.09 | 118.80      | 126.75   |
| 3   | K     | 601  | ADP  | C5-C4-N3 | -6.08 | 118.82      | 126.75   |
| 3   | D     | 1600 | ADP  | C5-C4-N3 | -6.07 | 118.83      | 126.75   |
| 3   | M     | 601  | ADP  | C5-C4-N3 | -6.05 | 118.86      | 126.75   |
| 3   | C     | 1600 | ADP  | C5-C4-N3 | -6.02 | 118.89      | 126.75   |
| 3   | G     | 1600 | ADP  | C5-C4-N3 | -6.02 | 118.90      | 126.75   |
| 3   | A     | 1600 | ADP  | C5-C4-N3 | -5.97 | 118.96      | 126.75   |
| 3   | L     | 601  | ADP  | C5-C4-N3 | -5.95 | 118.98      | 126.75   |
| 3   | F     | 1600 | ADP  | C5-C4-N3 | -5.92 | 119.02      | 126.75   |
| 3   | B     | 1600 | ADP  | C5-C4-N3 | -5.81 | 119.16      | 126.75   |
| 3   | J     | 601  | ADP  | N3-C4-N9 | 4.90  | 135.16      | 127.08   |
| 3   | H     | 601  | ADP  | N3-C4-N9 | 4.83  | 135.04      | 127.08   |
| 3   | M     | 601  | ADP  | N3-C4-N9 | 4.78  | 134.96      | 127.08   |
| 3   | C     | 1600 | ADP  | N3-C4-N9 | 4.77  | 134.94      | 127.08   |
| 3   | E     | 1600 | ADP  | N3-C4-N9 | 4.75  | 134.91      | 127.08   |
| 3   | N     | 601  | ADP  | N3-C4-N9 | 4.74  | 134.90      | 127.08   |
| 3   | I     | 601  | ADP  | N3-C4-N9 | 4.73  | 134.87      | 127.08   |
| 3   | K     | 601  | ADP  | N3-C4-N9 | 4.72  | 134.86      | 127.08   |
| 3   | A     | 1600 | ADP  | N3-C4-N9 | 4.66  | 134.75      | 127.08   |
| 3   | D     | 1600 | ADP  | N3-C4-N9 | 4.62  | 134.69      | 127.08   |
| 3   | L     | 601  | ADP  | N3-C4-N9 | 4.61  | 134.67      | 127.08   |
| 3   | F     | 1600 | ADP  | N3-C4-N9 | 4.57  | 134.62      | 127.08   |
| 3   | B     | 1600 | ADP  | N3-C4-N9 | 4.52  | 134.53      | 127.08   |
| 3   | G     | 1600 | ADP  | N3-C4-N9 | 4.51  | 134.52      | 127.08   |
| 3   | G     | 1600 | ADP  | C2-N3-C4 | 4.01  | 121.22      | 111.75   |
| 3   | D     | 1600 | ADP  | C2-N3-C4 | 3.97  | 121.13      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | E     | 1600 | ADP  | C2-N3-C4  | 3.95  | 121.09      | 111.75   |
| 3   | F     | 1600 | ADP  | C2-N3-C4  | 3.94  | 121.06      | 111.75   |
| 3   | A     | 1600 | ADP  | C2-N3-C4  | 3.88  | 120.92      | 111.75   |
| 3   | J     | 601  | ADP  | C2-N3-C4  | 3.87  | 120.90      | 111.75   |
| 3   | B     | 1600 | ADP  | C2-N3-C4  | 3.86  | 120.88      | 111.75   |
| 3   | C     | 1600 | ADP  | C2-N3-C4  | 3.86  | 120.86      | 111.75   |
| 3   | I     | 601  | ADP  | C2-N3-C4  | 3.85  | 120.84      | 111.75   |
| 3   | K     | 601  | ADP  | C2-N3-C4  | 3.84  | 120.82      | 111.75   |
| 3   | H     | 601  | ADP  | C2-N3-C4  | 3.83  | 120.81      | 111.75   |
| 3   | N     | 601  | ADP  | C2-N3-C4  | 3.82  | 120.78      | 111.75   |
| 3   | M     | 601  | ADP  | C2-N3-C4  | 3.82  | 120.78      | 111.75   |
| 3   | L     | 601  | ADP  | C2-N3-C4  | 3.79  | 120.71      | 111.75   |
| 3   | G     | 1600 | ADP  | N3-C2-N1  | -3.47 | 123.17      | 128.60   |
| 3   | F     | 1600 | ADP  | N3-C2-N1  | -3.47 | 123.17      | 128.60   |
| 3   | D     | 1600 | ADP  | C4-C5-N7  | -3.43 | 106.44      | 110.62   |
| 3   | G     | 1600 | ADP  | C4-C5-N7  | -3.42 | 106.45      | 110.62   |
| 3   | E     | 1600 | ADP  | N3-C2-N1  | -3.37 | 123.33      | 128.60   |
| 3   | I     | 601  | ADP  | C4-C5-N7  | -3.36 | 106.53      | 110.62   |
| 3   | D     | 1600 | ADP  | N3-C2-N1  | -3.35 | 123.37      | 128.60   |
| 3   | B     | 1600 | ADP  | N3-C2-N1  | -3.33 | 123.39      | 128.60   |
| 3   | F     | 1600 | ADP  | C4-C5-N7  | -3.33 | 106.57      | 110.62   |
| 3   | N     | 601  | ADP  | C4-C5-N7  | -3.32 | 106.57      | 110.62   |
| 3   | A     | 1600 | ADP  | N3-C2-N1  | -3.32 | 123.41      | 128.60   |
| 3   | B     | 1600 | ADP  | C4-C5-N7  | -3.32 | 106.58      | 110.62   |
| 3   | K     | 601  | ADP  | C4-C5-N7  | -3.30 | 106.60      | 110.62   |
| 3   | E     | 1600 | ADP  | C4-C5-N7  | -3.29 | 106.61      | 110.62   |
| 3   | C     | 1600 | ADP  | C4-C5-N7  | -3.28 | 106.62      | 110.62   |
| 3   | C     | 1600 | ADP  | N3-C2-N1  | -3.28 | 123.47      | 128.60   |
| 3   | L     | 601  | ADP  | C4-C5-N7  | -3.27 | 106.63      | 110.62   |
| 3   | J     | 601  | ADP  | C4-C5-N7  | -3.27 | 106.64      | 110.62   |
| 3   | H     | 601  | ADP  | C4-C5-N7  | -3.22 | 106.69      | 110.62   |
| 3   | A     | 1600 | ADP  | C4-C5-N7  | -3.22 | 106.69      | 110.62   |
| 3   | M     | 601  | ADP  | C4-C5-N7  | -3.22 | 106.70      | 110.62   |
| 3   | K     | 601  | ADP  | N3-C2-N1  | -3.19 | 123.61      | 128.60   |
| 3   | I     | 601  | ADP  | N3-C2-N1  | -3.19 | 123.62      | 128.60   |
| 3   | J     | 601  | ADP  | N3-C2-N1  | -3.18 | 123.62      | 128.60   |
| 3   | M     | 601  | ADP  | N3-C2-N1  | -3.17 | 123.64      | 128.60   |
| 3   | L     | 601  | ADP  | N3-C2-N1  | -3.16 | 123.66      | 128.60   |
| 3   | H     | 601  | ADP  | N3-C2-N1  | -3.16 | 123.66      | 128.60   |
| 3   | H     | 601  | ADP  | PA-O3A-PB | -3.15 | 122.00      | 132.83   |
| 3   | N     | 601  | ADP  | N3-C2-N1  | -3.14 | 123.69      | 128.60   |
| 3   | N     | 601  | ADP  | PA-O3A-PB | -3.10 | 122.19      | 132.83   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | M     | 601  | ADP  | PA-O3A-PB | -3.00 | 122.53      | 132.83   |
| 3   | K     | 601  | ADP  | PA-O3A-PB | -2.90 | 122.87      | 132.83   |
| 3   | L     | 601  | ADP  | PA-O3A-PB | -2.89 | 122.91      | 132.83   |
| 3   | I     | 601  | ADP  | PA-O3A-PB | -2.86 | 123.01      | 132.83   |
| 3   | J     | 601  | ADP  | PA-O3A-PB | -2.85 | 123.06      | 132.83   |
| 3   | J     | 601  | ADP  | C4-N9-C8  | 2.85  | 108.81      | 105.73   |
| 3   | B     | 1600 | ADP  | C4-N9-C8  | 2.83  | 108.79      | 105.73   |
| 3   | D     | 1600 | ADP  | C5-N7-C8  | 2.80  | 107.49      | 103.51   |
| 3   | F     | 1600 | ADP  | C5-N7-C8  | 2.78  | 107.46      | 103.51   |
| 3   | G     | 1600 | ADP  | C5-N7-C8  | 2.77  | 107.44      | 103.51   |
| 3   | M     | 601  | ADP  | C4-N9-C8  | 2.77  | 108.73      | 105.73   |
| 3   | C     | 1600 | ADP  | C4-N9-C8  | 2.77  | 108.72      | 105.73   |
| 3   | C     | 1600 | ADP  | C5-N7-C8  | 2.76  | 107.43      | 103.51   |
| 3   | F     | 1600 | ADP  | C4-N9-C8  | 2.75  | 108.71      | 105.73   |
| 3   | B     | 1600 | ADP  | C5-N7-C8  | 2.74  | 107.40      | 103.51   |
| 3   | A     | 1600 | ADP  | C4-N9-C8  | 2.74  | 108.69      | 105.73   |
| 3   | K     | 601  | ADP  | C4-N9-C8  | 2.73  | 108.69      | 105.73   |
| 3   | J     | 601  | ADP  | C5-N7-C8  | 2.73  | 107.39      | 103.51   |
| 3   | I     | 601  | ADP  | C5-N7-C8  | 2.72  | 107.38      | 103.51   |
| 3   | K     | 601  | ADP  | C5-N7-C8  | 2.72  | 107.37      | 103.51   |
| 3   | N     | 601  | ADP  | C5-N7-C8  | 2.72  | 107.37      | 103.51   |
| 3   | I     | 601  | ADP  | C4-N9-C8  | 2.71  | 108.67      | 105.73   |
| 3   | M     | 601  | ADP  | C5-N7-C8  | 2.70  | 107.35      | 103.51   |
| 3   | E     | 1600 | ADP  | C5-N7-C8  | 2.70  | 107.34      | 103.51   |
| 3   | H     | 601  | ADP  | C5-N7-C8  | 2.69  | 107.33      | 103.51   |
| 3   | D     | 1600 | ADP  | C4-N9-C8  | 2.69  | 108.64      | 105.73   |
| 3   | N     | 601  | ADP  | C4-N9-C8  | 2.68  | 108.64      | 105.73   |
| 3   | L     | 601  | ADP  | C4-N9-C8  | 2.67  | 108.63      | 105.73   |
| 3   | L     | 601  | ADP  | C5-N7-C8  | 2.67  | 107.30      | 103.51   |
| 3   | H     | 601  | ADP  | C4-N9-C8  | 2.64  | 108.59      | 105.73   |
| 3   | A     | 1600 | ADP  | C5-N7-C8  | 2.63  | 107.25      | 103.51   |
| 3   | E     | 1600 | ADP  | C4-N9-C8  | 2.61  | 108.55      | 105.73   |
| 3   | G     | 1600 | ADP  | C4-N9-C8  | 2.56  | 108.50      | 105.73   |
| 3   | G     | 1600 | ADP  | C6-C5-N7  | 2.52  | 136.72      | 132.02   |
| 3   | B     | 1600 | ADP  | C6-C5-N7  | 2.47  | 136.63      | 132.02   |
| 3   | D     | 1600 | ADP  | C6-C5-N7  | 2.47  | 136.63      | 132.02   |
| 3   | F     | 1600 | ADP  | C6-C5-N7  | 2.46  | 136.60      | 132.02   |
| 3   | E     | 1600 | ADP  | C6-C5-N7  | 2.35  | 136.40      | 132.02   |
| 3   | A     | 1600 | ADP  | C6-C5-N7  | 2.33  | 136.37      | 132.02   |
| 3   | C     | 1600 | ADP  | C6-C5-N7  | 2.29  | 136.29      | 132.02   |
| 3   | L     | 601  | ADP  | C6-C5-N7  | 2.24  | 136.20      | 132.02   |
| 3   | I     | 601  | ADP  | C6-C5-N7  | 2.23  | 136.18      | 132.02   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | A     | 1600 | ADP  | O3B-PB-O2B | 2.22  | 116.14      | 107.64   |
| 3   | N     | 601  | ADP  | C6-C5-N7   | 2.22  | 136.16      | 132.02   |
| 3   | C     | 1600 | ADP  | O3B-PB-O2B | 2.21  | 116.10      | 107.64   |
| 3   | F     | 1600 | ADP  | N9-C8-N7   | -2.20 | 110.90      | 113.91   |
| 3   | M     | 601  | ADP  | C6-C5-N7   | 2.20  | 136.12      | 132.02   |
| 3   | B     | 1600 | ADP  | N9-C8-N7   | -2.18 | 110.93      | 113.91   |
| 3   | K     | 601  | ADP  | C6-C5-N7   | 2.18  | 136.09      | 132.02   |
| 3   | J     | 601  | ADP  | C6-C5-N7   | 2.18  | 136.08      | 132.02   |
| 3   | D     | 1600 | ADP  | N9-C8-N7   | -2.17 | 110.95      | 113.91   |
| 3   | H     | 601  | ADP  | C6-C5-N7   | 2.15  | 136.02      | 132.02   |
| 3   | F     | 1600 | ADP  | O3B-PB-O2B | 2.14  | 115.81      | 107.64   |
| 3   | J     | 601  | ADP  | N9-C8-N7   | -2.12 | 111.02      | 113.91   |
| 3   | K     | 601  | ADP  | N9-C8-N7   | -2.11 | 111.02      | 113.91   |
| 3   | G     | 1600 | ADP  | N9-C8-N7   | -2.11 | 111.03      | 113.91   |
| 3   | M     | 601  | ADP  | N9-C8-N7   | -2.10 | 111.04      | 113.91   |
| 3   | C     | 1600 | ADP  | N9-C8-N7   | -2.09 | 111.06      | 113.91   |
| 3   | G     | 1600 | ADP  | O3B-PB-O2B | 2.08  | 115.60      | 107.64   |
| 3   | A     | 1600 | ADP  | N9-C8-N7   | -2.07 | 111.08      | 113.91   |
| 3   | E     | 1600 | ADP  | O3B-PB-O2B | 2.06  | 115.52      | 107.64   |
| 3   | L     | 601  | ADP  | N9-C8-N7   | -2.06 | 111.09      | 113.91   |
| 3   | I     | 601  | ADP  | N9-C8-N7   | -2.06 | 111.10      | 113.91   |
| 3   | N     | 601  | ADP  | N9-C8-N7   | -2.06 | 111.10      | 113.91   |
| 3   | B     | 1600 | ADP  | PA-O3A-PB  | -2.03 | 125.86      | 132.83   |
| 3   | E     | 1600 | ADP  | N9-C8-N7   | -2.00 | 111.17      | 113.91   |
| 3   | B     | 1600 | ADP  | O3B-PB-O2B | 2.00  | 115.28      | 107.64   |

There are no chirality outliers.

All (107) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | A     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | A     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | B     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | B     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | B     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | B     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | C     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | C     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | C     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | D     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | D     | 1600 | ADP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | E     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | E     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | E     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | E     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | F     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | F     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | G     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | G     | 1600 | ADP  | C5'-O5'-PA-O1A  |
| 3   | G     | 1600 | ADP  | C5'-O5'-PA-O2A  |
| 3   | G     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | H     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | H     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | I     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | I     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | I     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | J     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | J     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | K     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | K     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | K     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | L     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | L     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | L     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | M     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | M     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | M     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | N     | 601  | ADP  | C5'-O5'-PA-O2A  |
| 3   | N     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | F     | 1600 | ADP  | C3'-C4'-C5'-O5' |
| 3   | H     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | J     | 601  | ADP  | C3'-C4'-C5'-O5' |
| 3   | A     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | B     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | C     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | M     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | D     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | E     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | I     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | K     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | F     | 1600 | ADP  | O4'-C4'-C5'-O5' |
| 3   | G     | 1600 | ADP  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | H     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | J     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | L     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | N     | 601  | ADP  | O4'-C4'-C5'-O5' |
| 3   | A     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | B     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | E     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | F     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | G     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | C     | 1600 | ADP  | PA-O3A-PB-O1B   |
| 3   | F     | 1600 | ADP  | PA-O3A-PB-O1B   |
| 3   | A     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | C     | 1600 | ADP  | C5'-O5'-PA-O3A  |
| 3   | D     | 1600 | ADP  | C5'-O5'-PA-O3A  |
| 3   | G     | 1600 | ADP  | C5'-O5'-PA-O3A  |
| 3   | J     | 601  | ADP  | C5'-O5'-PA-O3A  |
| 3   | N     | 601  | ADP  | C5'-O5'-PA-O3A  |
| 3   | D     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | H     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | I     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | K     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | M     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | N     | 601  | ADP  | C5'-O5'-PA-O1A  |
| 3   | A     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | B     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | C     | 1600 | ADP  | PB-O3A-PA-O1A   |
| 3   | C     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | E     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | F     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | G     | 1600 | ADP  | PB-O3A-PA-O2A   |
| 3   | I     | 601  | ADP  | PB-O3A-PA-O1A   |
| 3   | J     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | L     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | N     | 601  | ADP  | PB-O3A-PA-O2A   |
| 3   | H     | 601  | ADP  | PB-O3A-PA-O1A   |
| 3   | K     | 601  | ADP  | PB-O3A-PA-O1A   |
| 3   | C     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | C     | 1600 | ADP  | PA-O3A-PB-O3B   |
| 3   | F     | 1600 | ADP  | PA-O3A-PB-O2B   |
| 3   | F     | 1600 | ADP  | PA-O3A-PB-O3B   |
| 3   | A     | 1600 | ADP  | C5'-O5'-PA-O3A  |
| 3   | B     | 1600 | ADP  | C5'-O5'-PA-O3A  |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | E     | 1600 | ADP  | C5'-O5'-PA-O3A |
| 3   | F     | 1600 | ADP  | C5'-O5'-PA-O3A |
| 3   | H     | 601  | ADP  | C5'-O5'-PA-O3A |
| 3   | I     | 601  | ADP  | C5'-O5'-PA-O3A |
| 3   | K     | 601  | ADP  | C5'-O5'-PA-O3A |
| 3   | L     | 601  | ADP  | C5'-O5'-PA-O3A |
| 3   | M     | 601  | ADP  | C5'-O5'-PA-O3A |
| 3   | J     | 601  | ADP  | PB-O3A-PA-O1A  |
| 3   | L     | 601  | ADP  | PB-O3A-PA-O1A  |
| 3   | M     | 601  | ADP  | PB-O3A-PA-O1A  |
| 3   | N     | 601  | ADP  | PB-O3A-PA-O1A  |

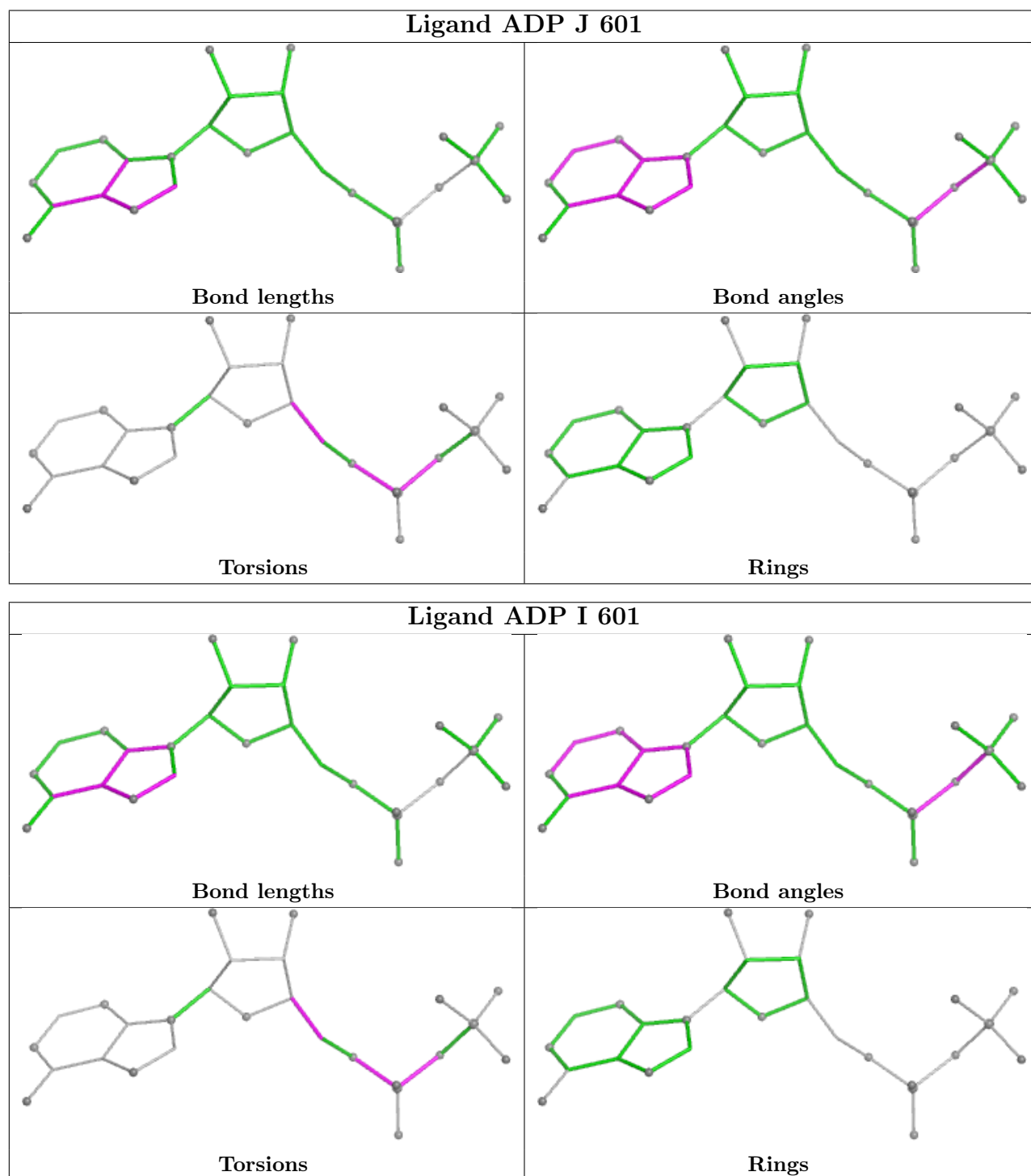
There are no ring outliers.

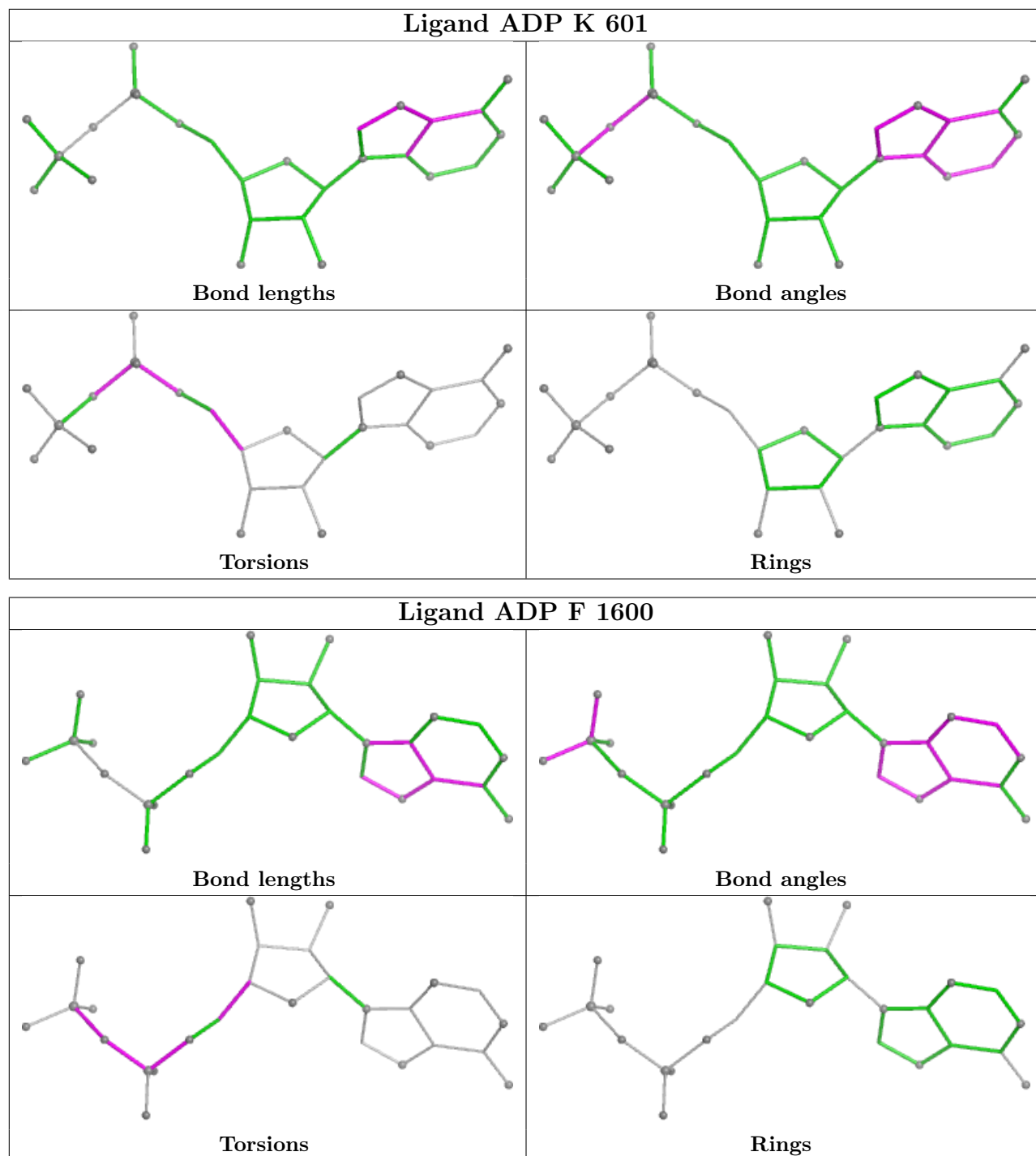
19 monomers are involved in 18 short contacts:

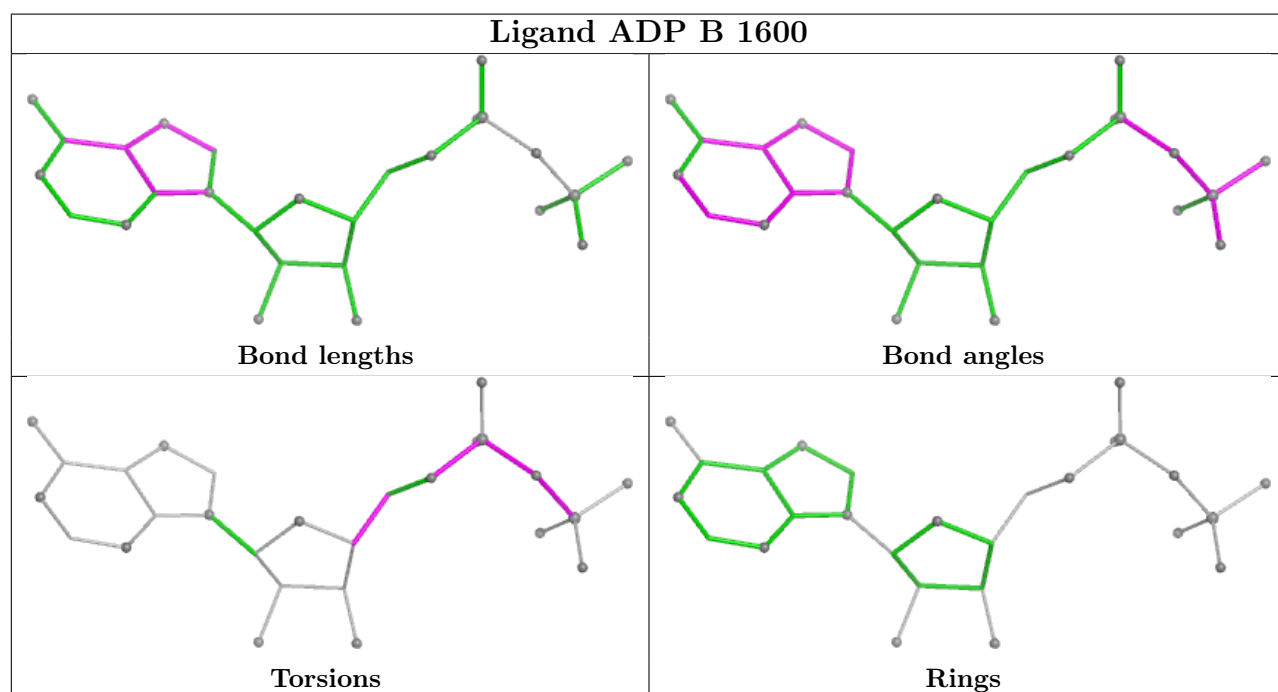
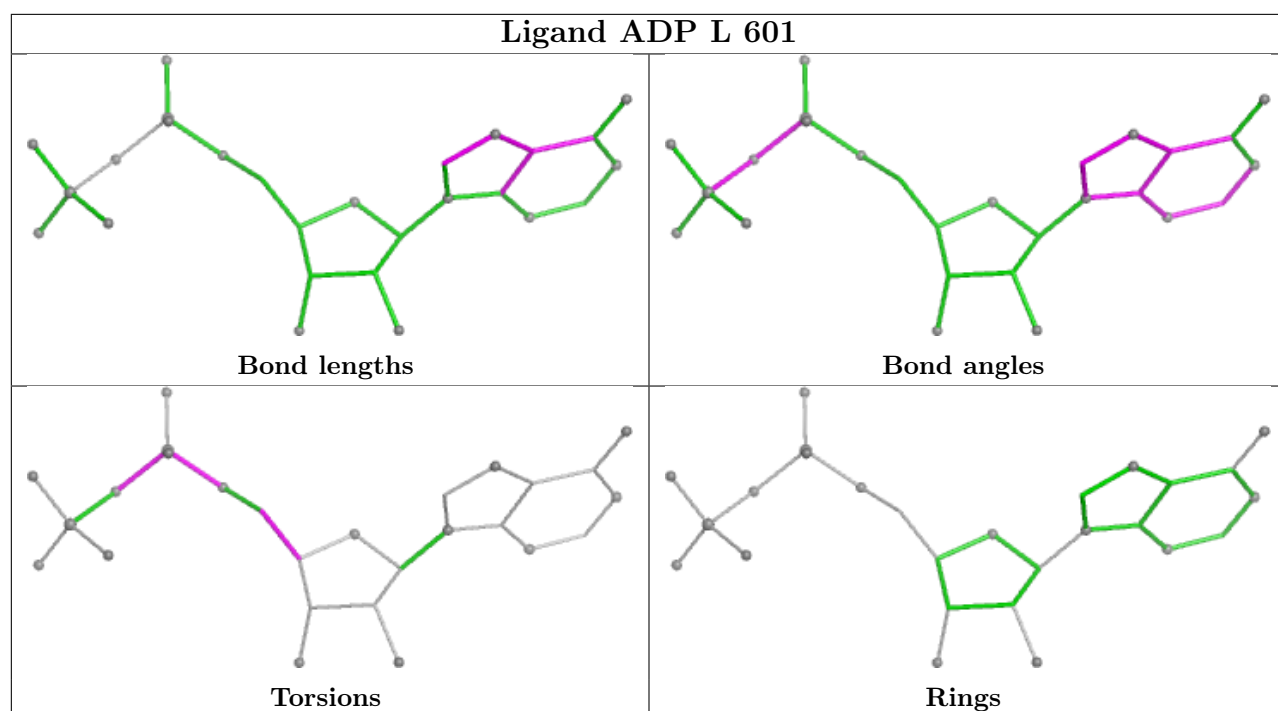
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | J     | 601  | ADP  | 1       | 0            |
| 3   | I     | 601  | ADP  | 1       | 0            |
| 3   | K     | 601  | ADP  | 1       | 0            |
| 5   | C     | 1602 | BEF  | 2       | 0            |
| 3   | F     | 1600 | ADP  | 2       | 0            |
| 3   | L     | 601  | ADP  | 1       | 0            |
| 3   | B     | 1600 | ADP  | 1       | 0            |
| 3   | C     | 1600 | ADP  | 3       | 0            |
| 5   | F     | 1602 | BEF  | 2       | 0            |
| 3   | G     | 1600 | ADP  | 2       | 0            |
| 3   | H     | 601  | ADP  | 1       | 0            |
| 3   | D     | 1600 | ADP  | 2       | 0            |
| 5   | D     | 1602 | BEF  | 1       | 0            |
| 5   | G     | 1602 | BEF  | 1       | 0            |
| 5   | E     | 1602 | BEF  | 1       | 0            |
| 3   | N     | 601  | ADP  | 1       | 0            |
| 5   | A     | 1602 | BEF  | 1       | 0            |
| 3   | E     | 1600 | ADP  | 1       | 0            |
| 3   | A     | 1600 | ADP  | 1       | 0            |

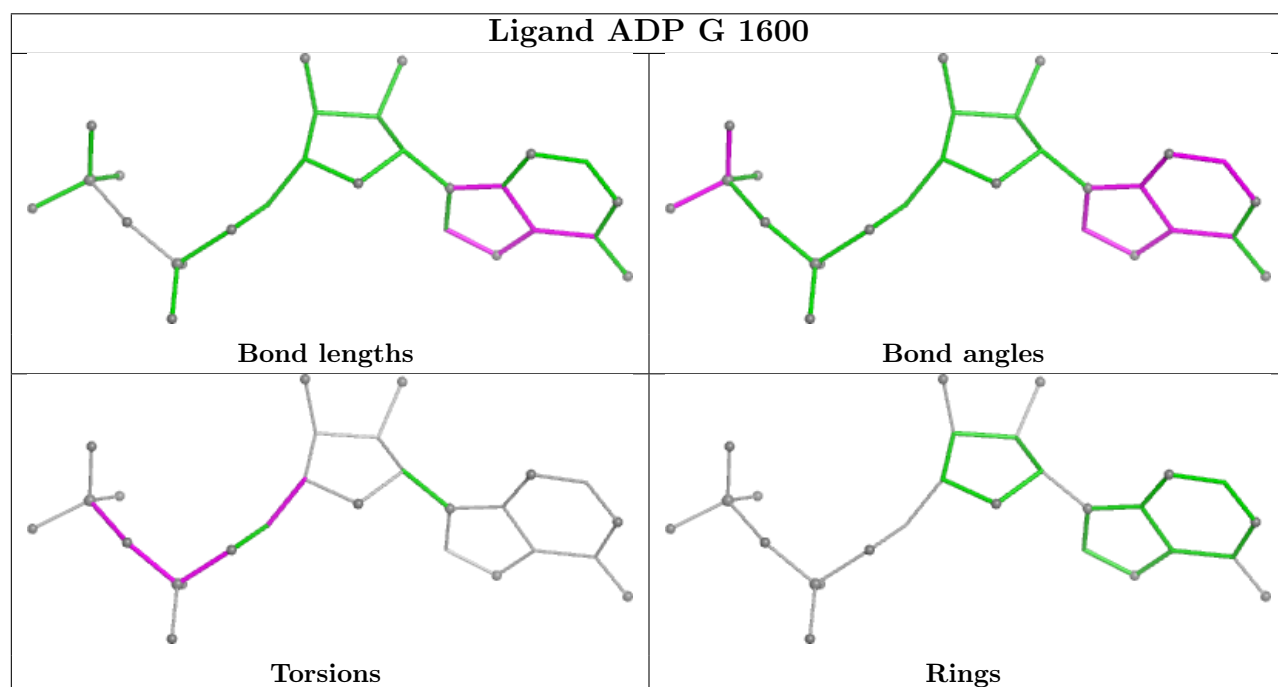
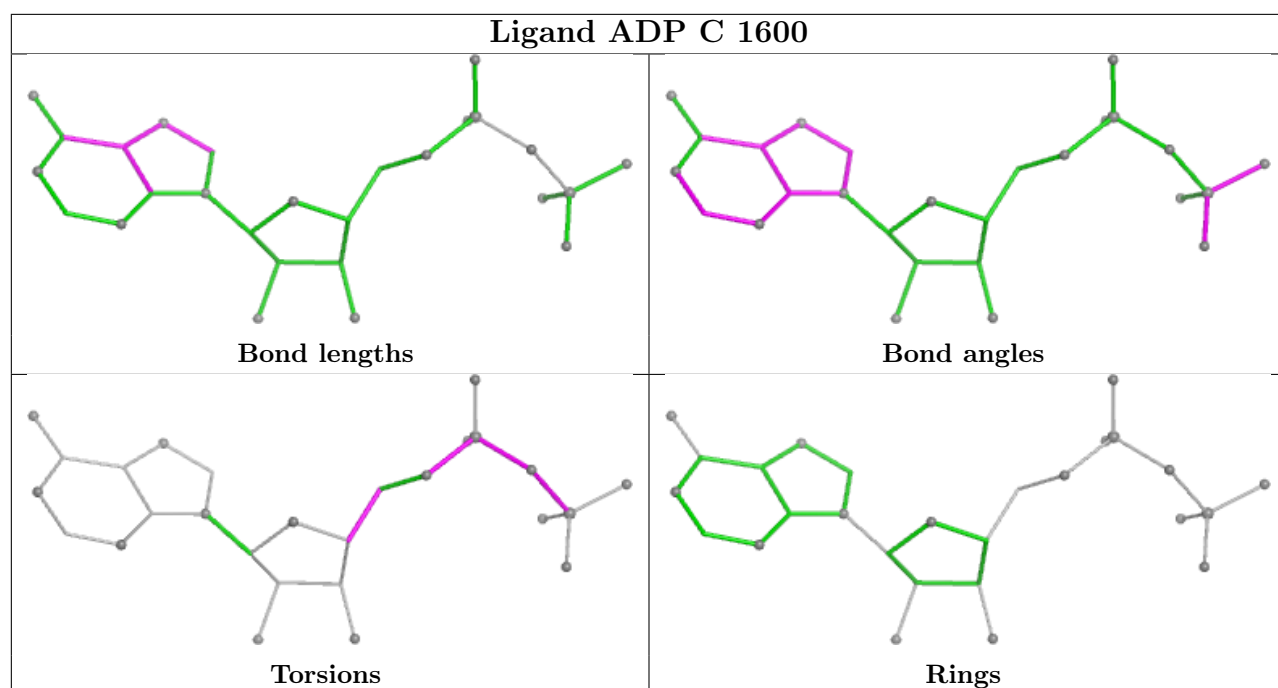
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

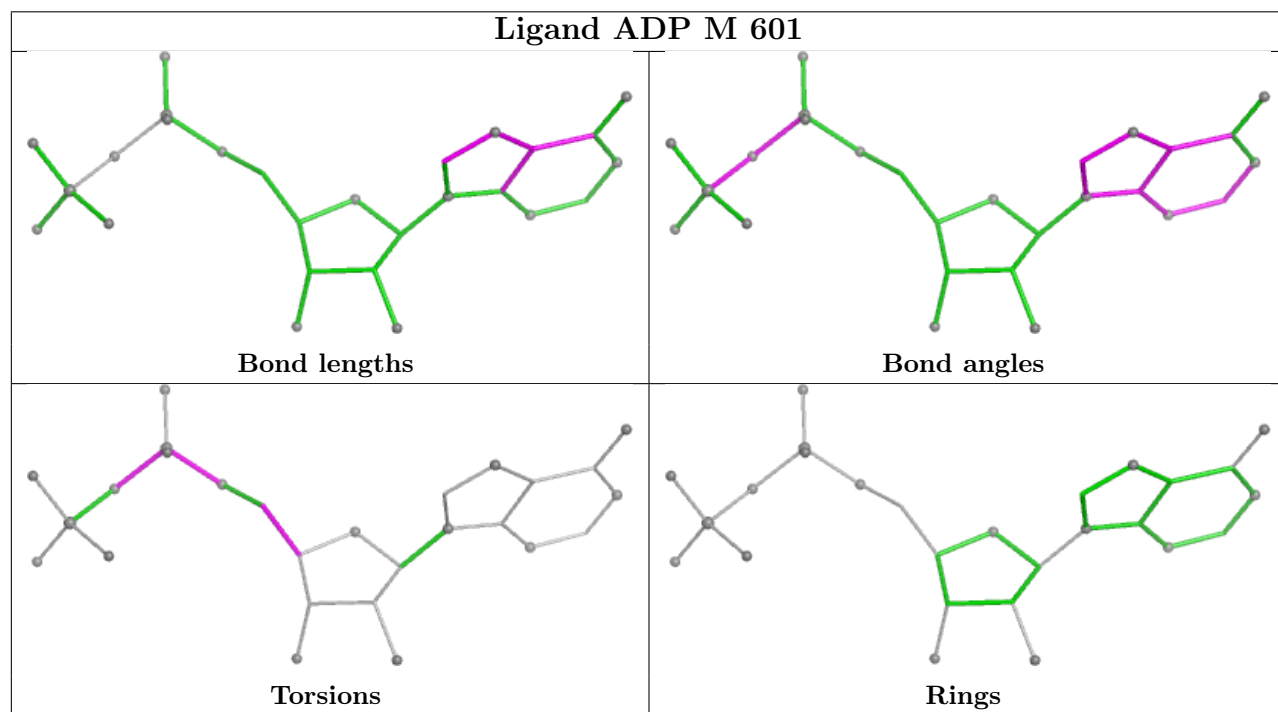
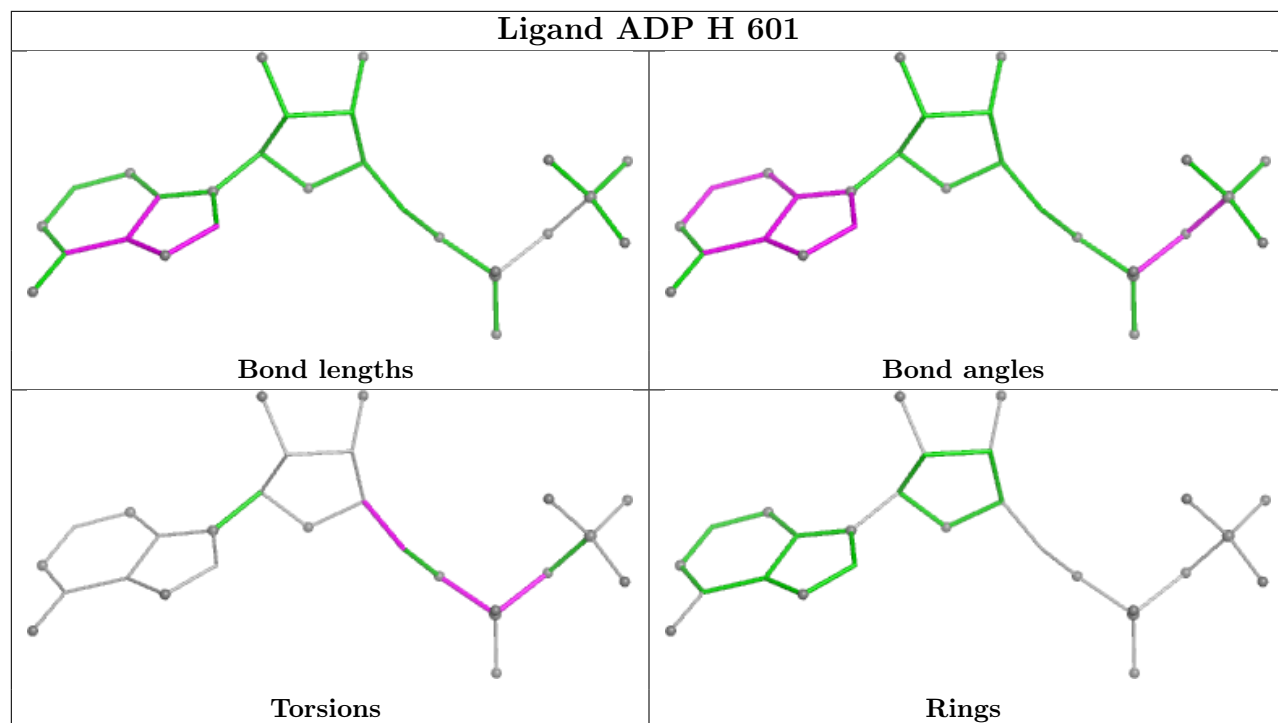
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

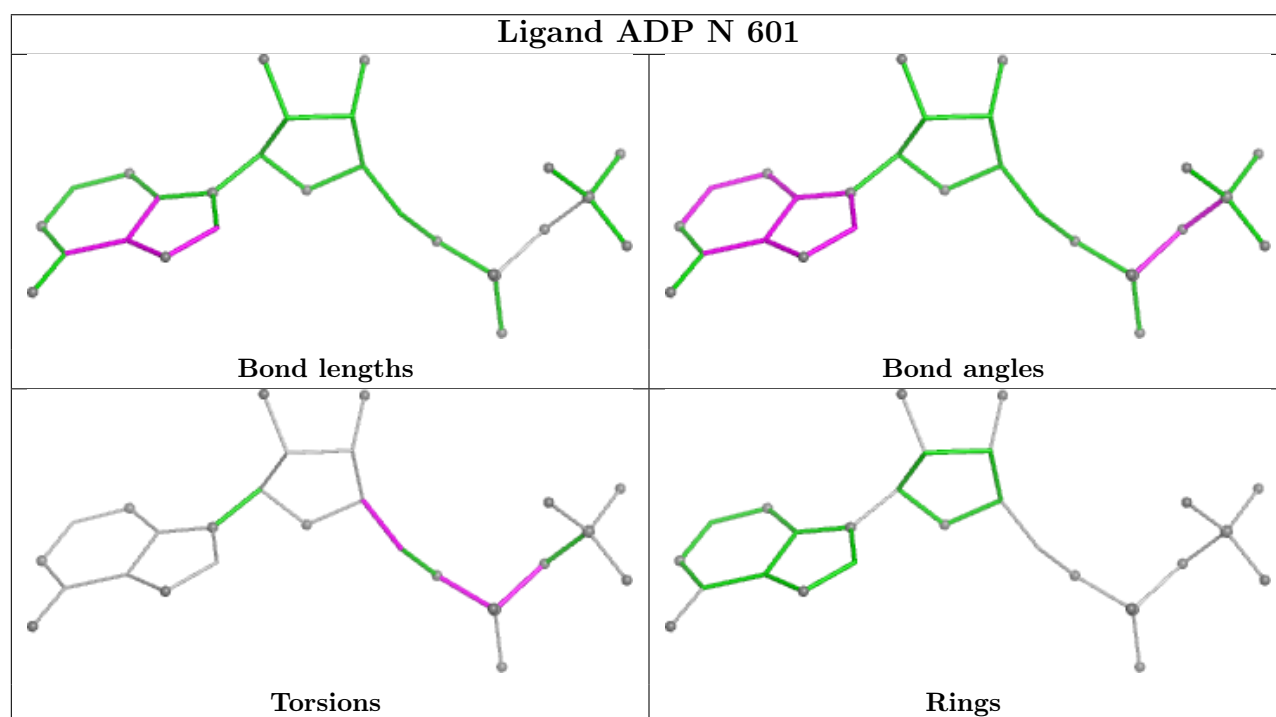
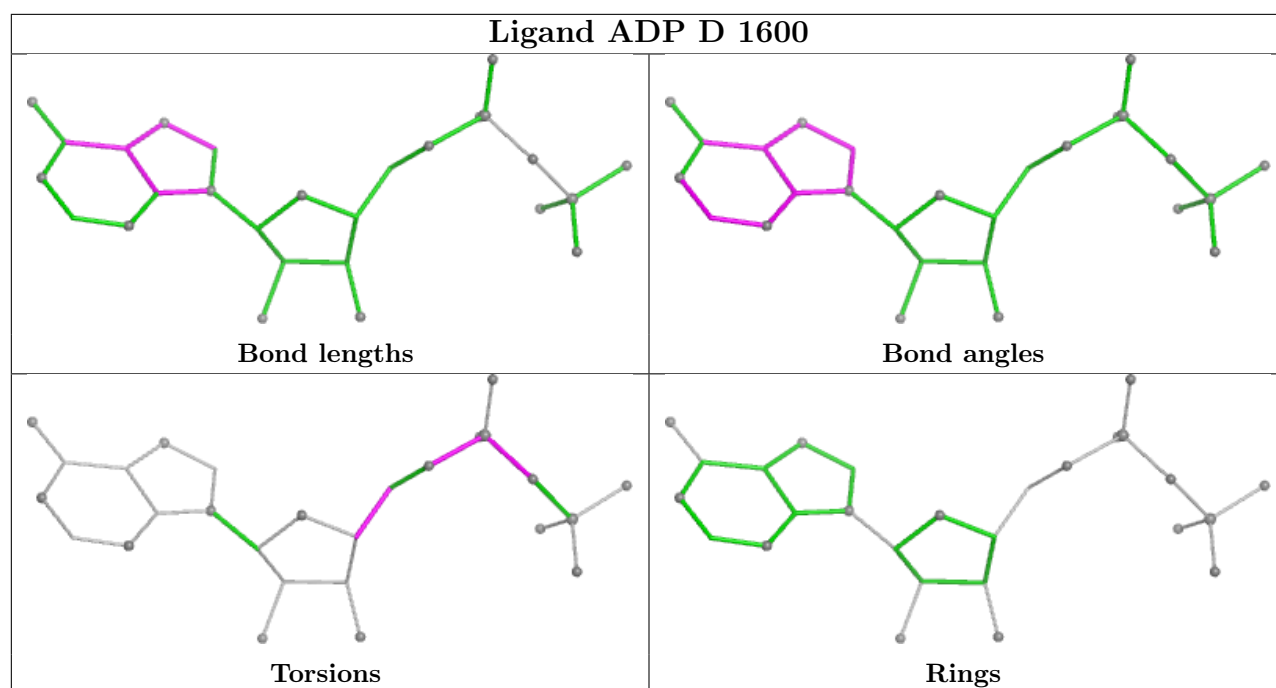


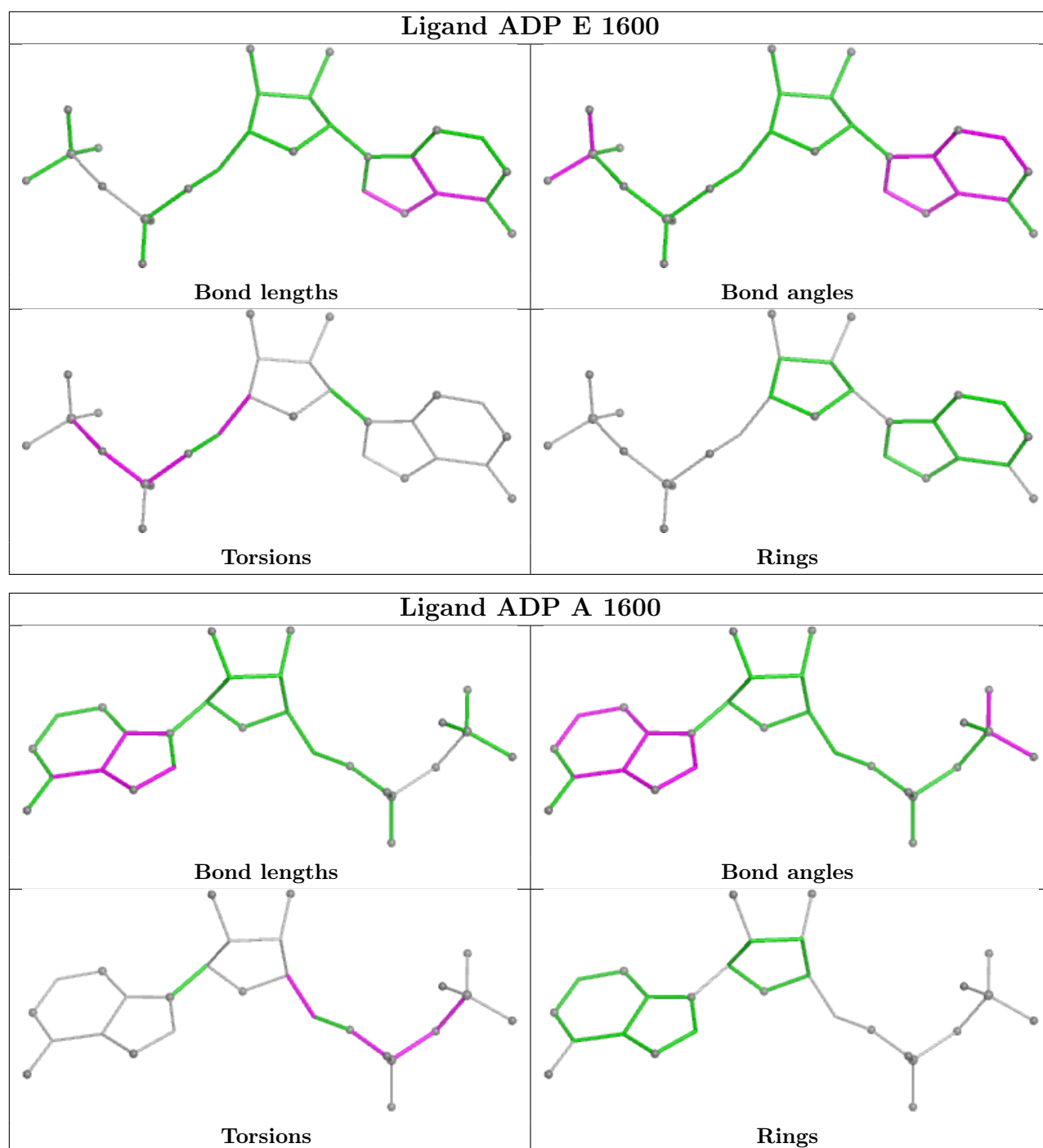












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

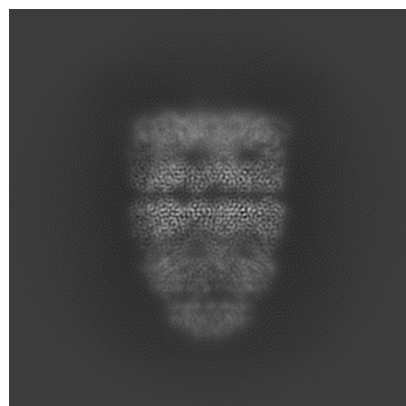
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18736. These allow visual inspection of the internal detail of the map and identification of artifacts.

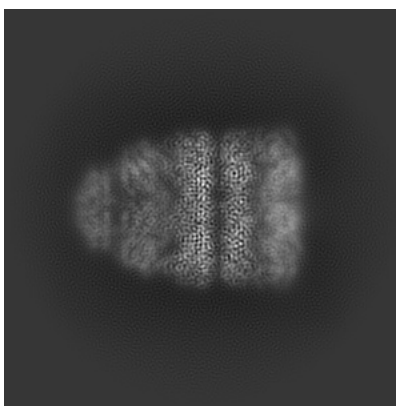
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

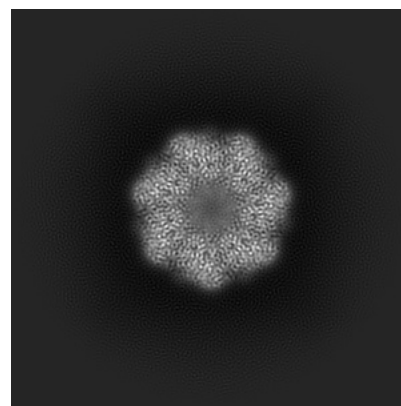
#### 6.1.1 Primary map



X

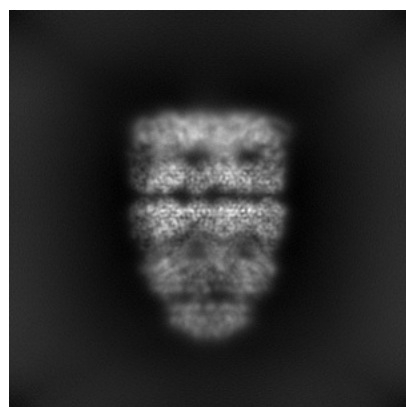


Y

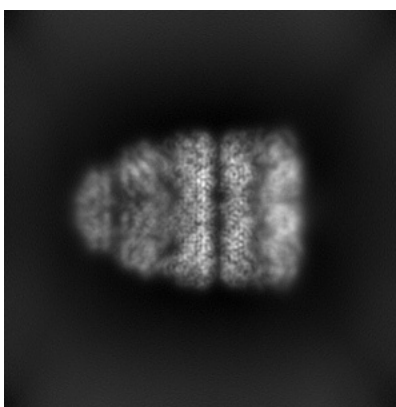


Z

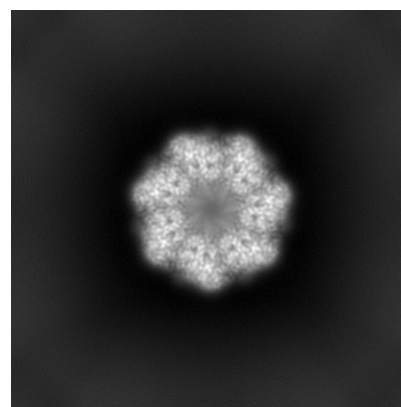
#### 6.1.2 Raw map



X



Y

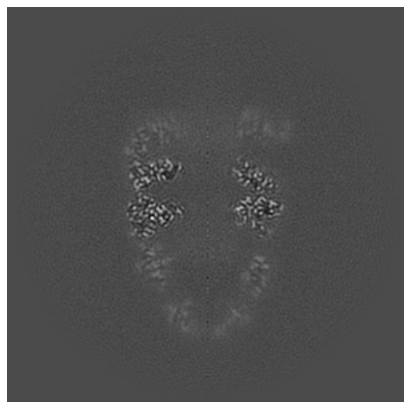


Z

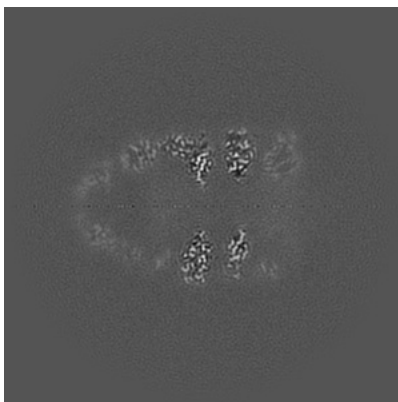
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

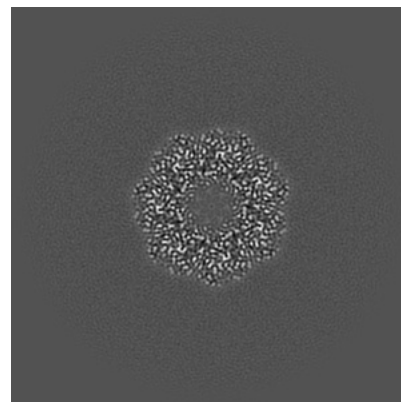
### 6.2.1 Primary map



X Index: 162

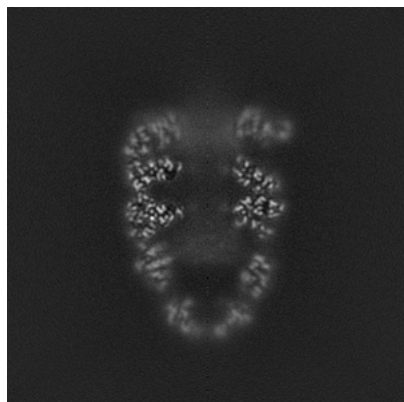


Y Index: 162

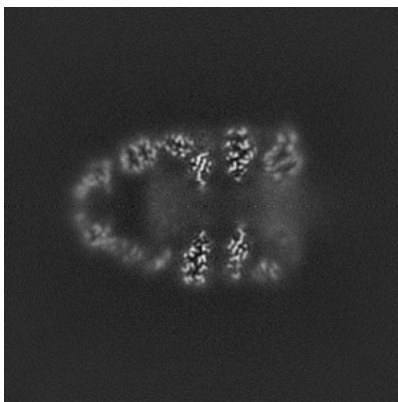


Z Index: 162

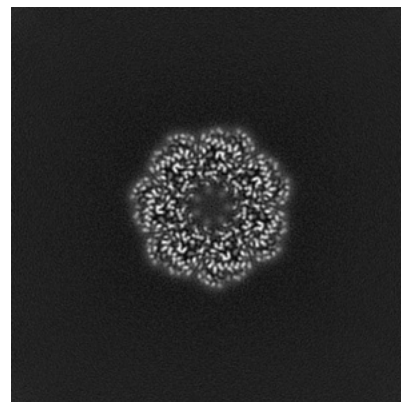
### 6.2.2 Raw map



X Index: 162



Y Index: 162

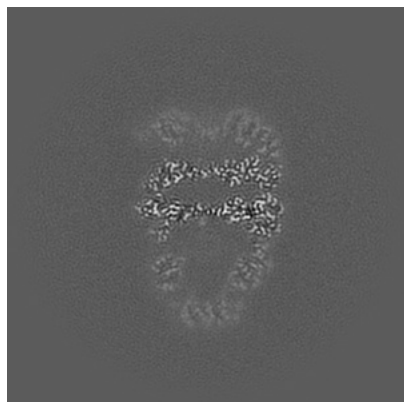


Z Index: 162

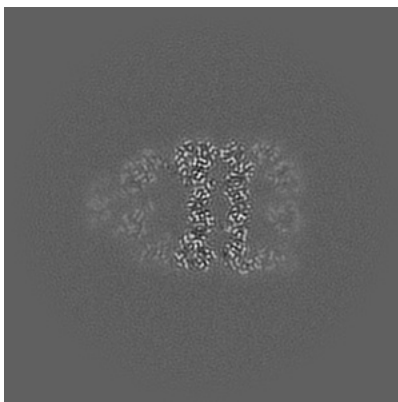
The images above show central slices of the map in three orthogonal directions.

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

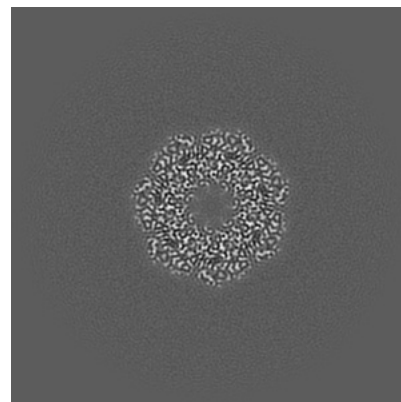
### 6.3.1 Primary map



X Index: 185

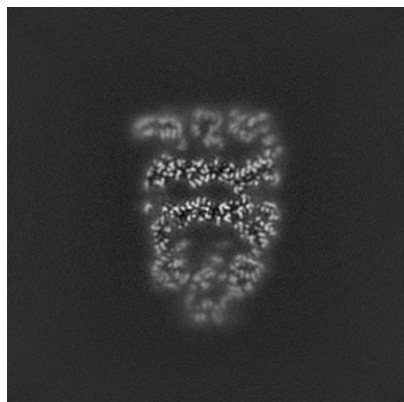


Y Index: 131

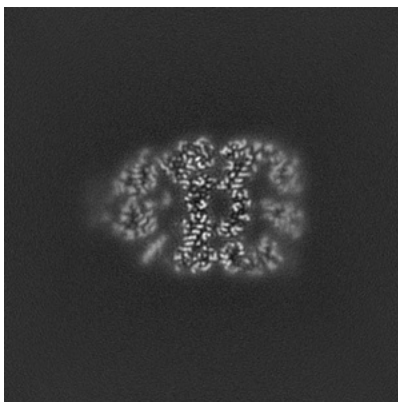


Z Index: 161

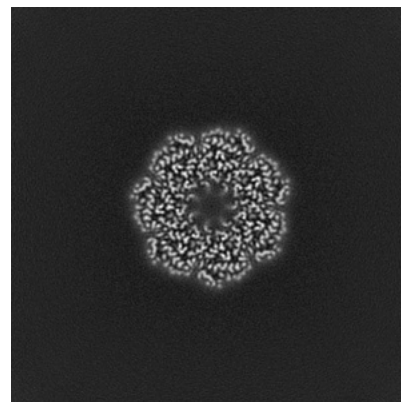
### 6.3.2 Raw map



X Index: 193



Y Index: 126

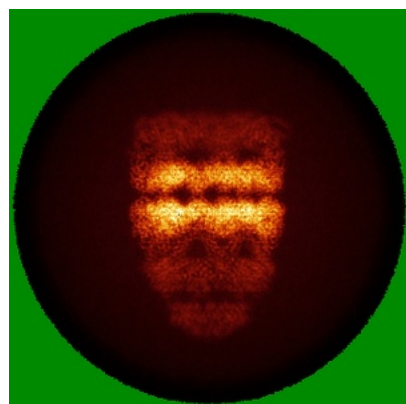


Z Index: 161

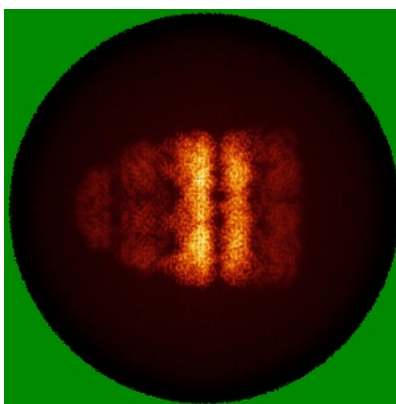
The images above show the largest variance slices of the map in three orthogonal directions.

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

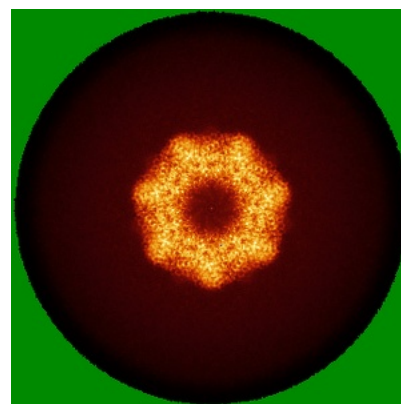
### 6.4.1 Primary map



X

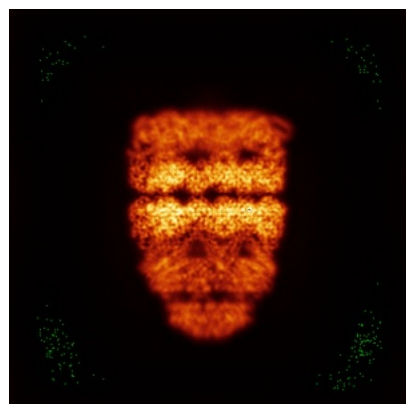


Y

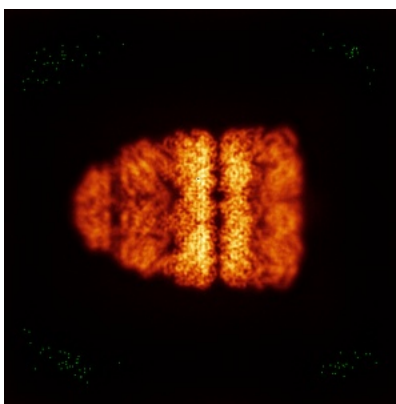


Z

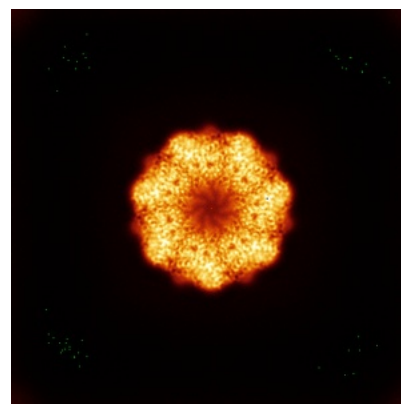
### 6.4.2 Raw map



X



Y

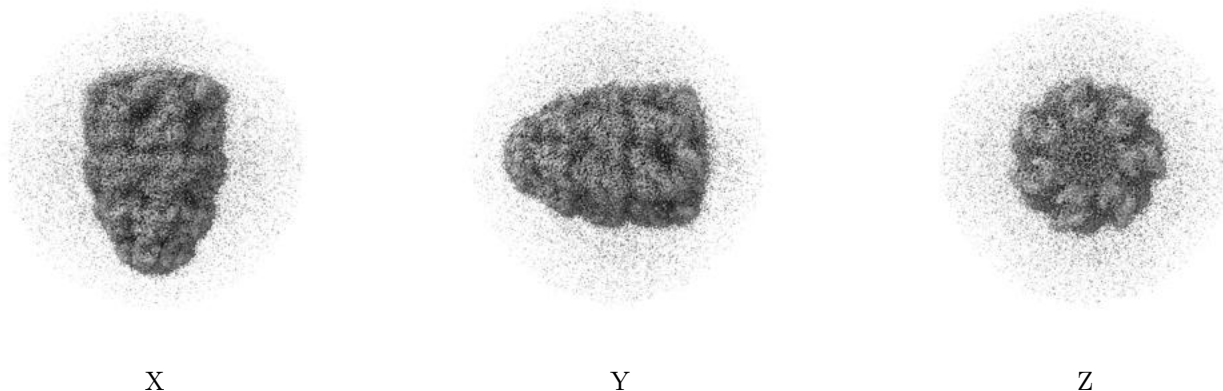


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

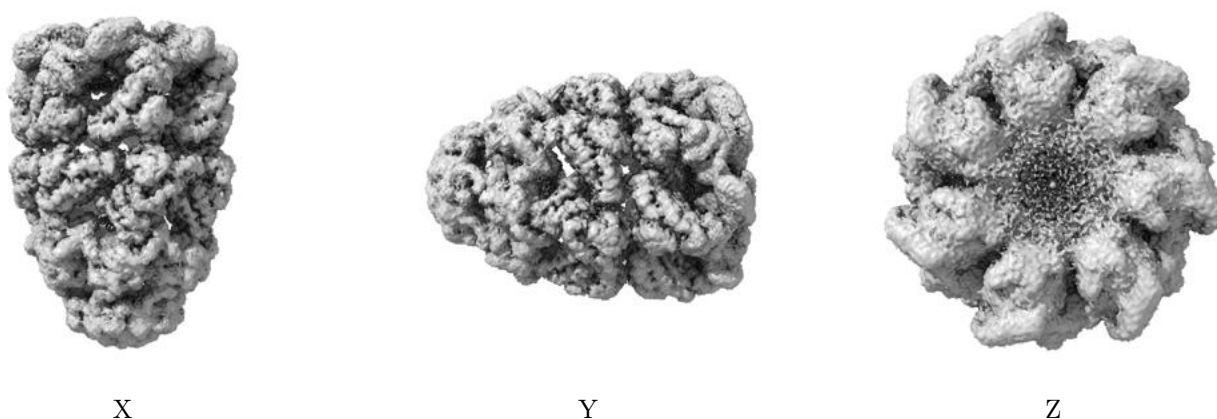
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.268. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

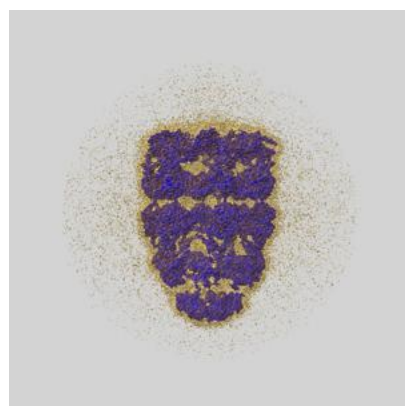
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

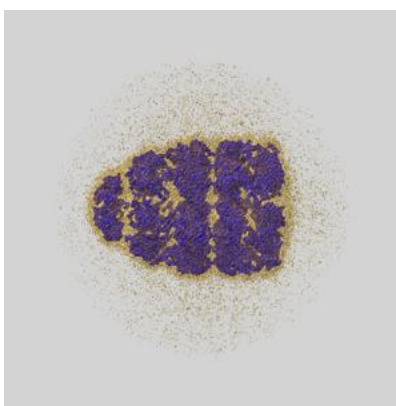
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

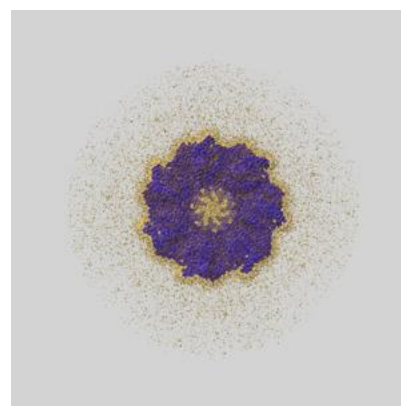
### 6.6.1 emd\_18736\_msk\_1.map [i](#)



X



Y

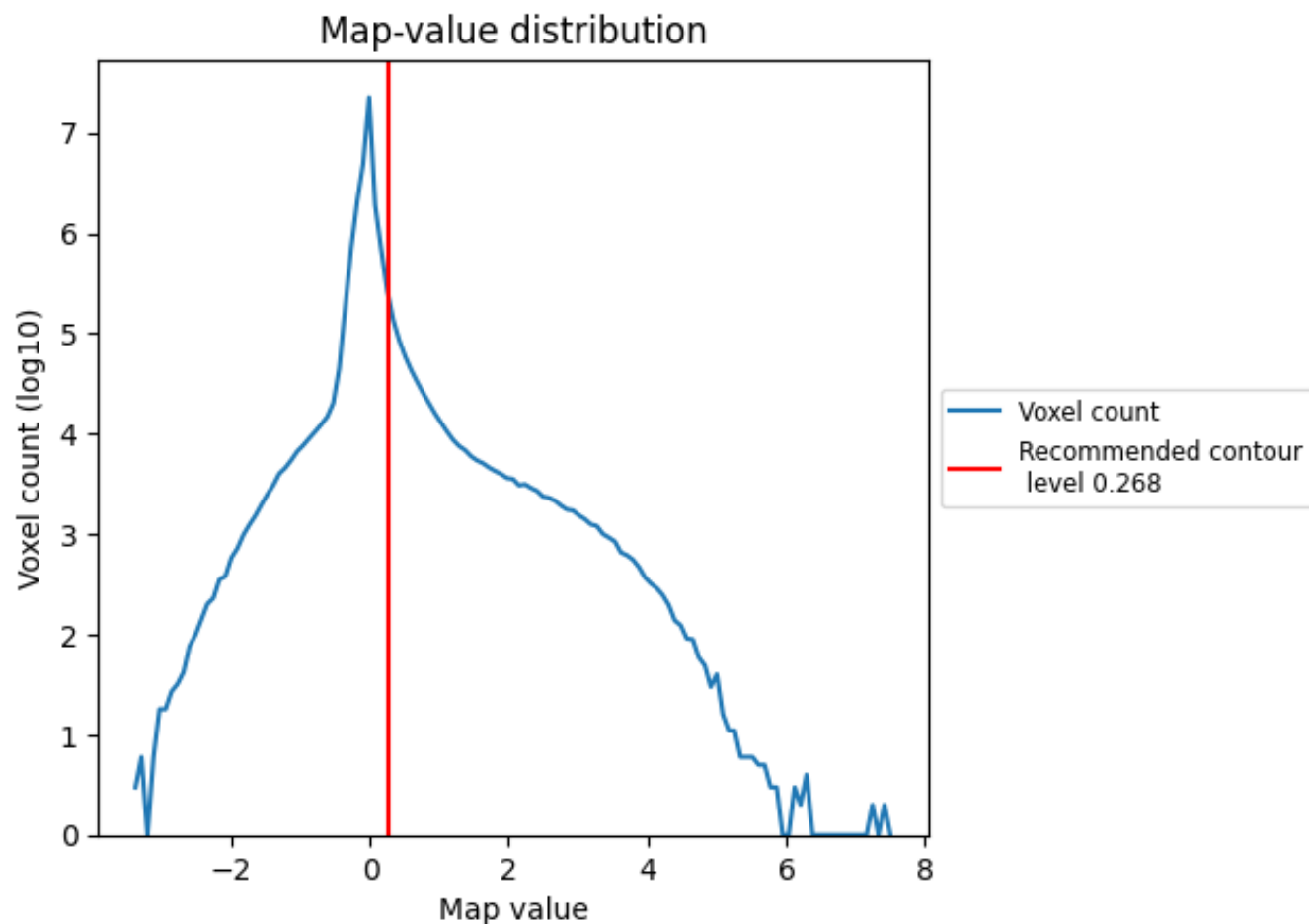


Z

## 7 Map analysis [i](#)

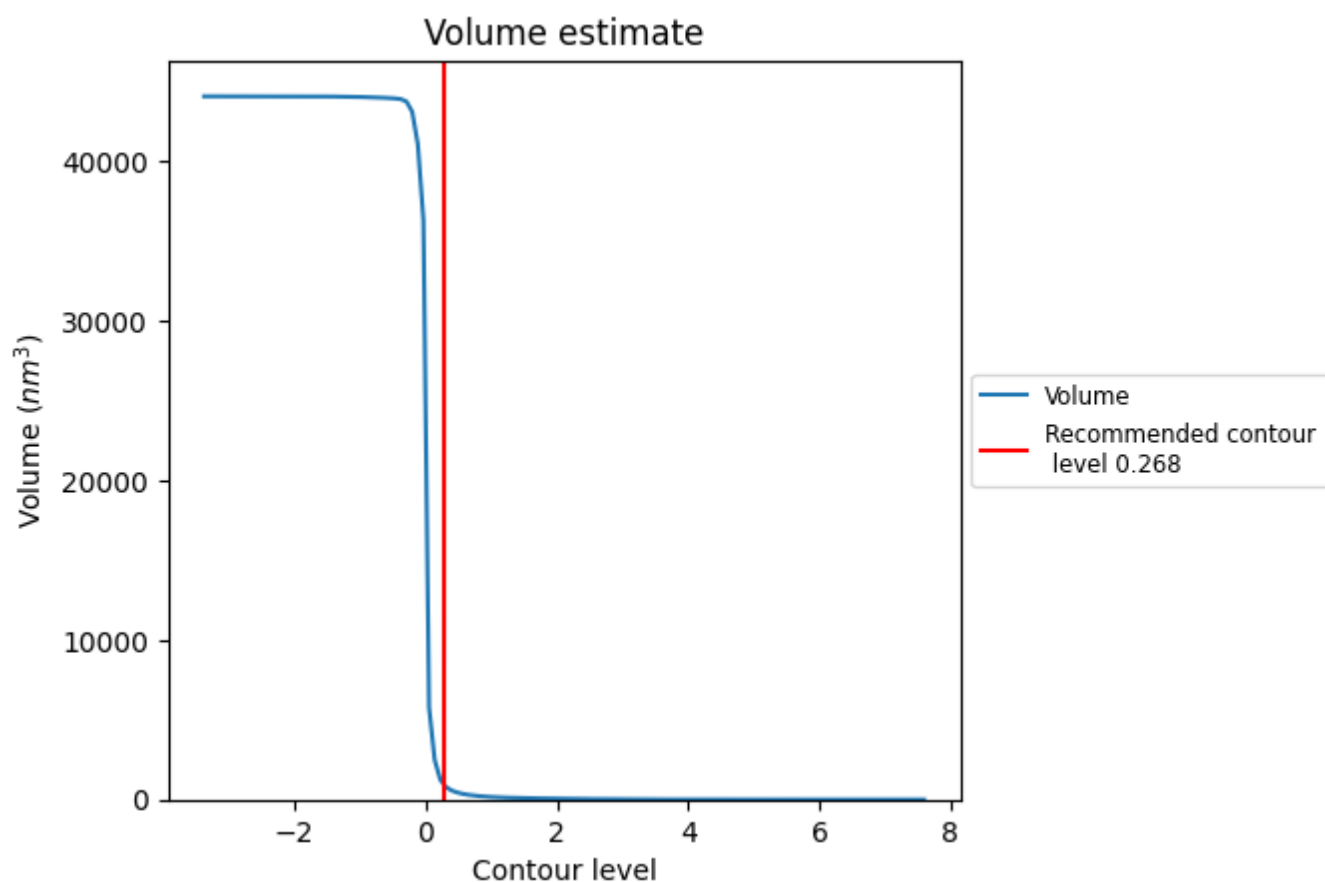
This section contains the results of statistical analysis of the map.

### 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.

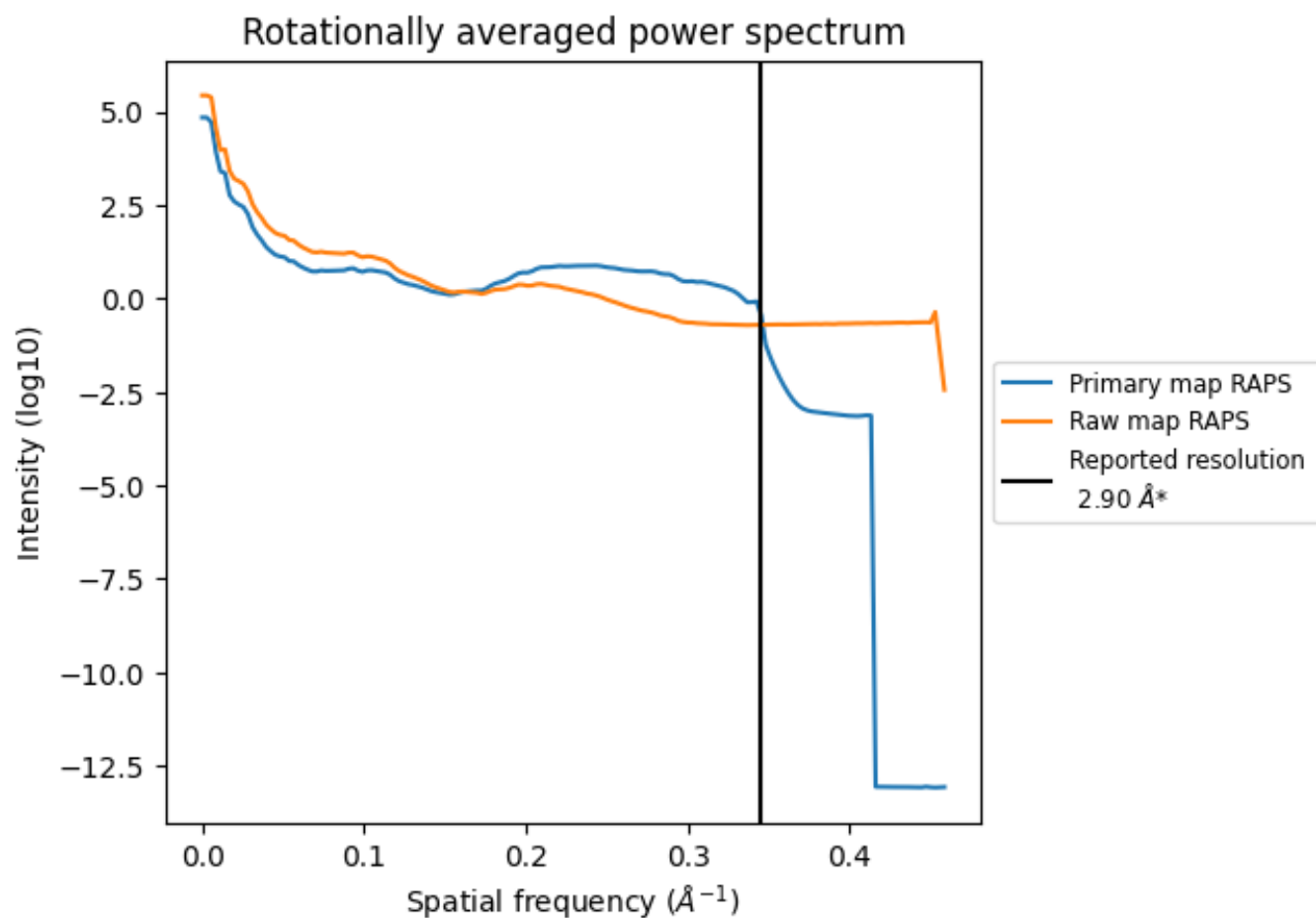
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 994 nm<sup>3</sup>; this corresponds to an approximate mass of 898 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 ⓘ

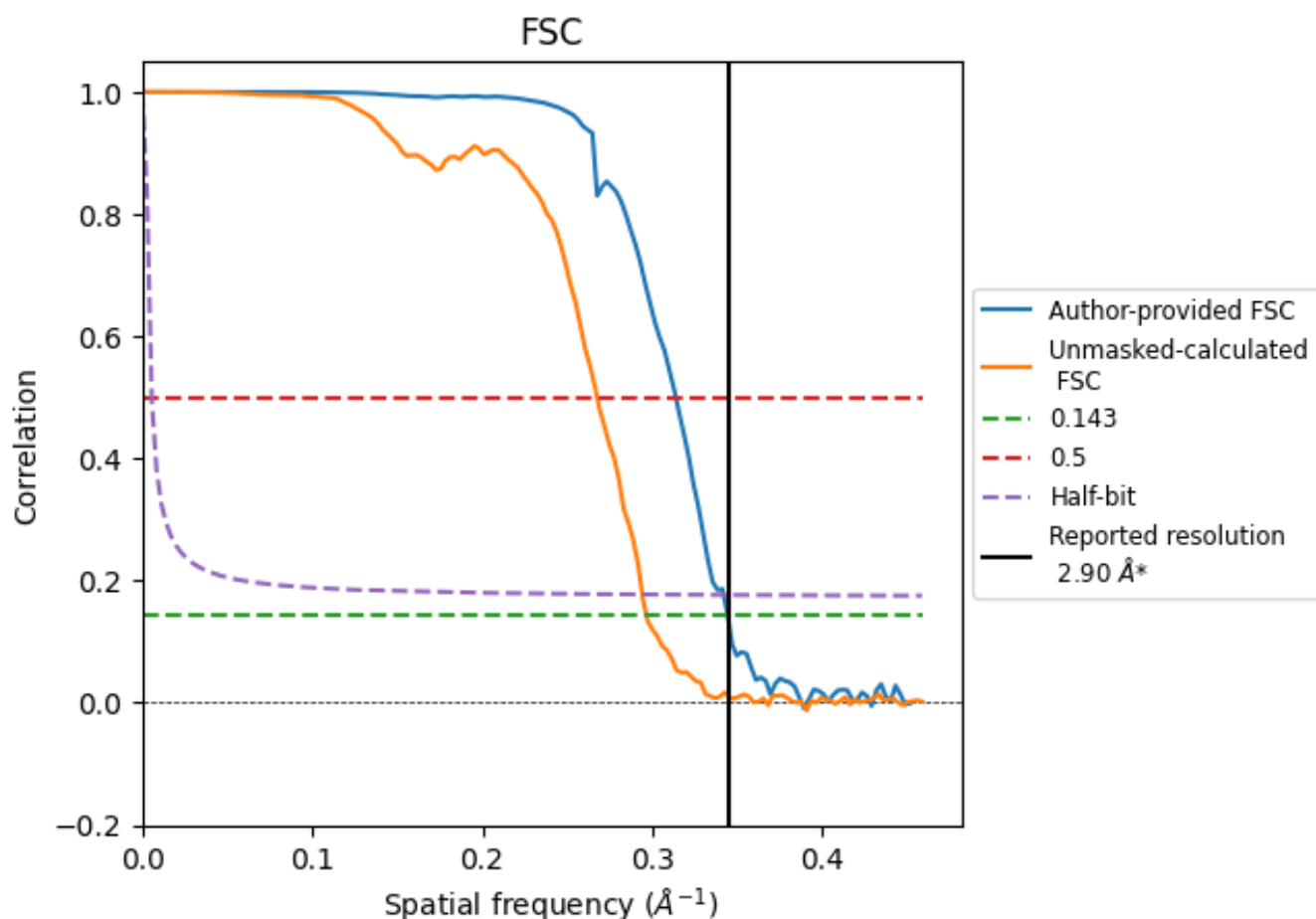


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

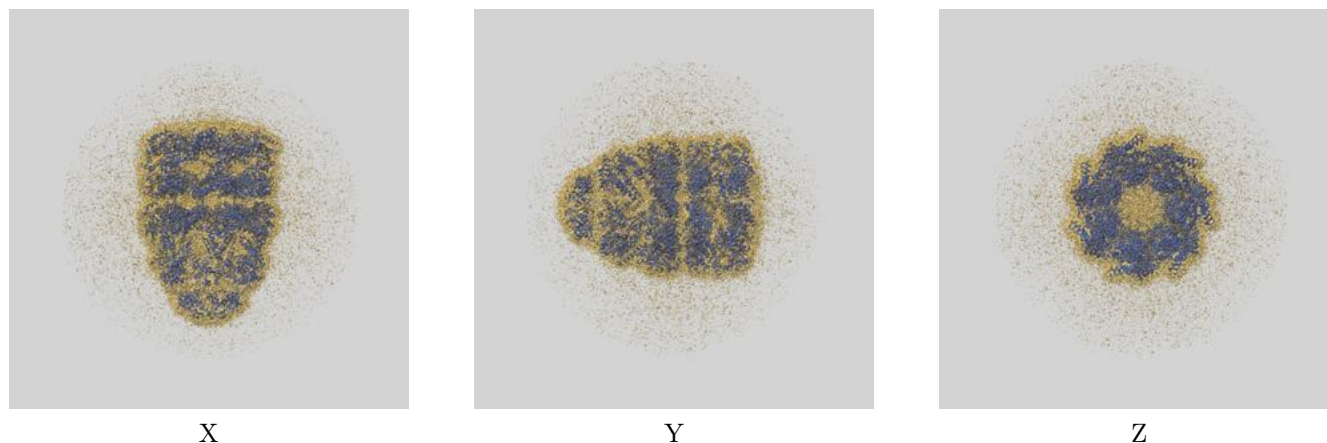
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.90                               | 3.19 | 2.92     |
| Unmasked-calculated*      | 3.37                               | 3.74 | 3.40     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.9 by more than 10 %

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

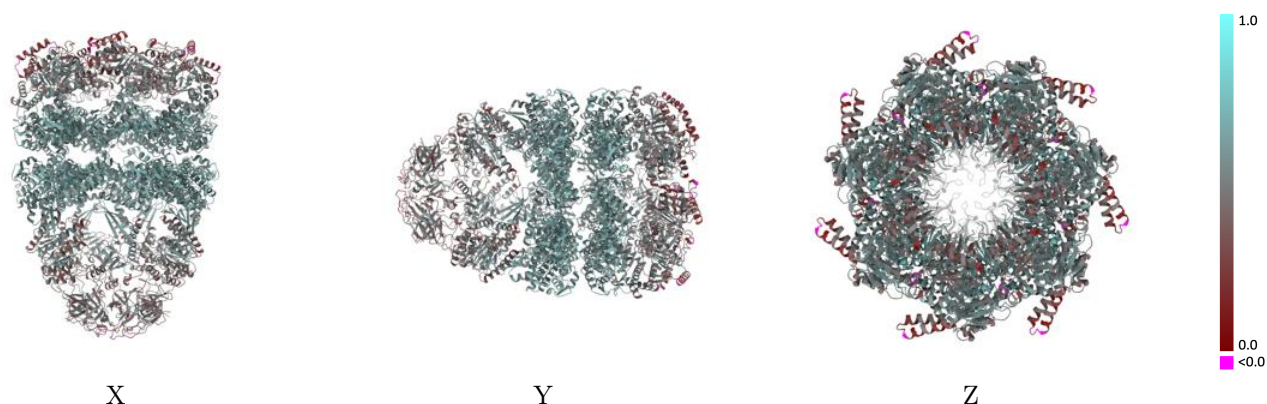
This section contains information regarding the fit between EMDB map EMD-18736 and PDB model 8QXT. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



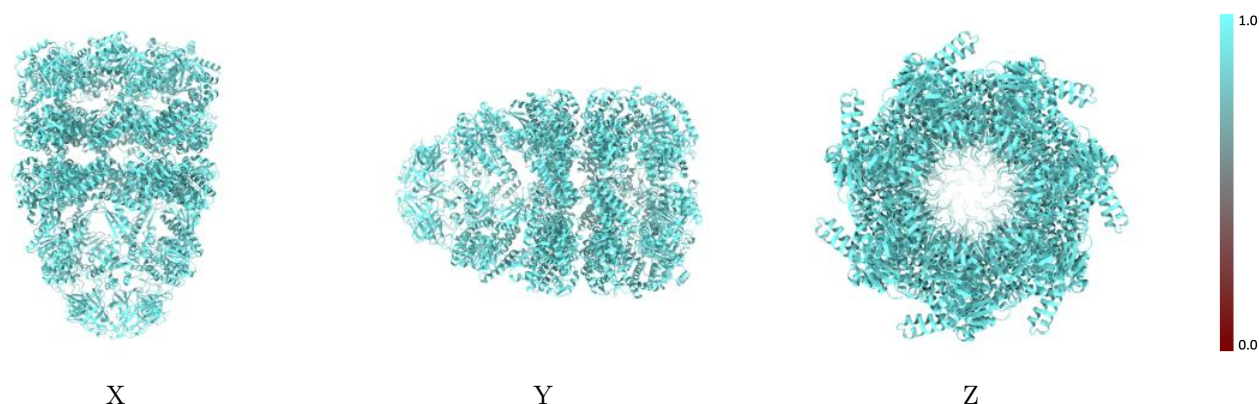
The images above show the 3D surface view of the map at the recommended contour level 0.268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



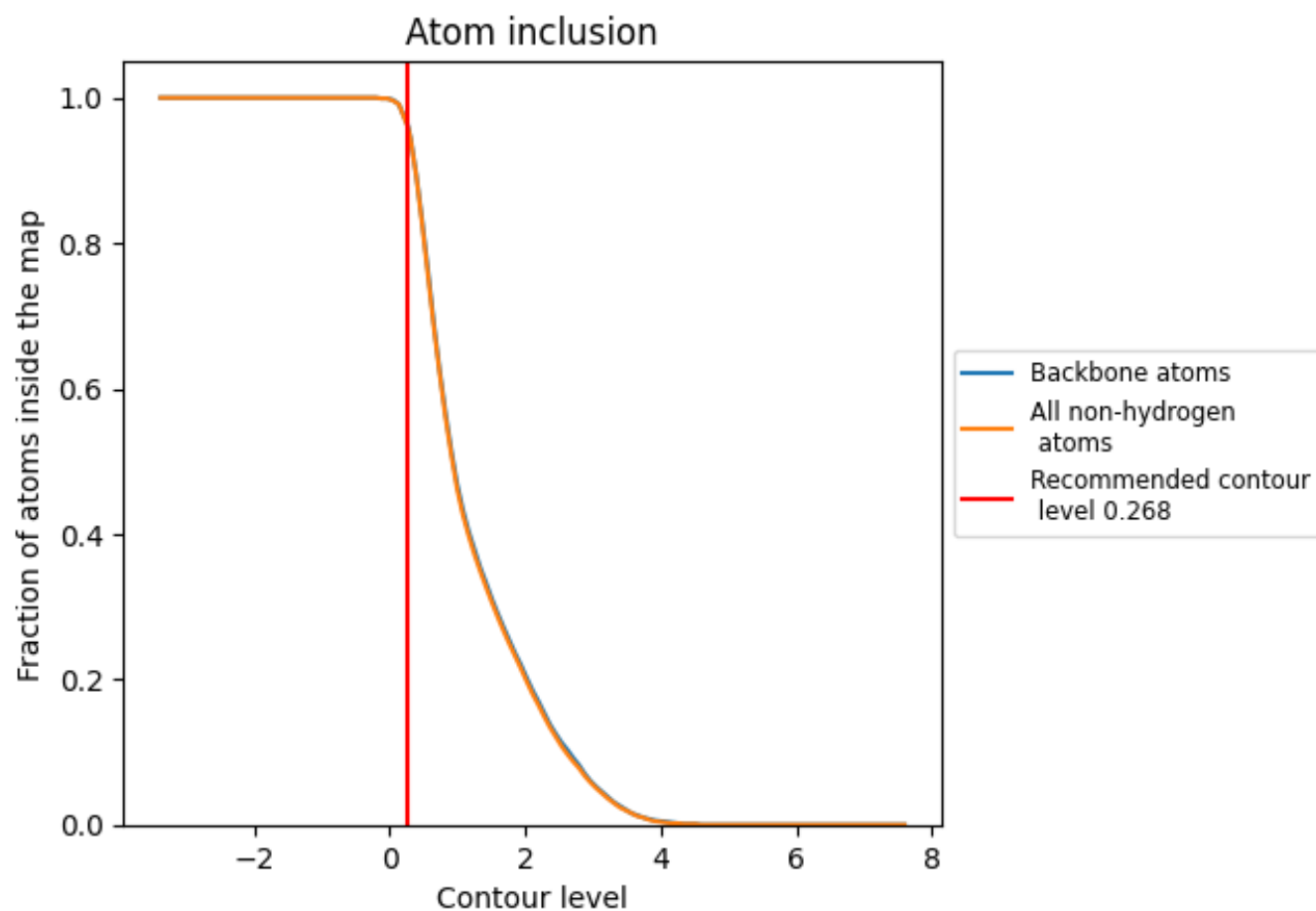
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.268).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.268) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9600   |  0.5150   |
| A     |  0.9640   |  0.5450   |
| B     |  0.9630   |  0.5440   |
| C     |  0.9610   |  0.5440   |
| D     |  0.9630   |  0.5460   |
| E     |  0.9640   |  0.5460   |
| F     |  0.9650   |  0.5460   |
| G     |  0.9620   |  0.5440   |
| H     |  0.9620   |  0.5050   |
| I     |  0.9590   |  0.5010   |
| J     |  0.9620   |  0.5020   |
| K     |  0.9590   |  0.5030   |
| L     |  0.9580   |  0.5010   |
| M     |  0.9570   |  0.5020   |
| N     |  0.9610  |  0.5030  |
| O     |  0.9590 |  0.4150 |
| P     |  0.9620 |  0.4140 |
| Q     |  0.9500 |  0.4070 |
| R     |  0.9540 |  0.4140 |
| S     |  0.9560 |  0.4150 |
| T     |  0.9530 |  0.4090 |
| U     |  0.9660 |  0.4100 |

