



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:19 AM UTC

PDB ID : 8BLC / pdb\_00008blc  
EMDB ID : EMD-16106  
Title : Structure of the GroEL-ATP complex plunge-frozen 50 ms after mixing with ATP  
Authors : Dhurandhar, M.; Torino, S.; Efremov, R.  
Deposited on : 2022-11-09  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

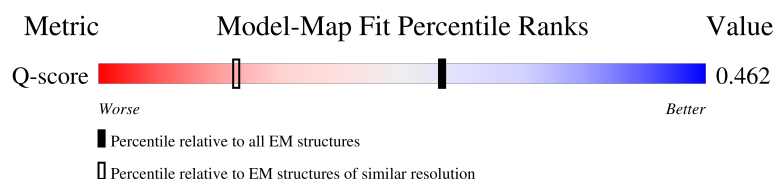
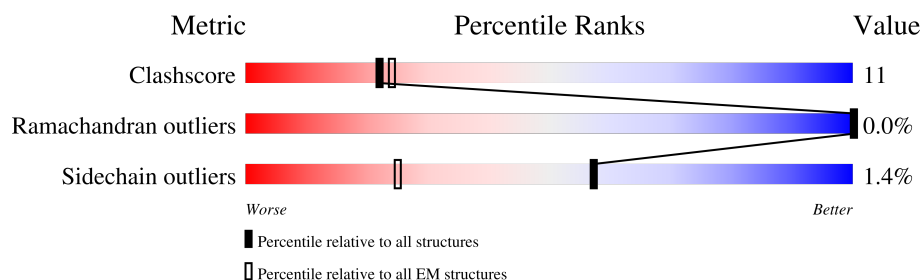
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.



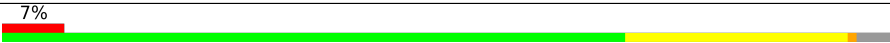
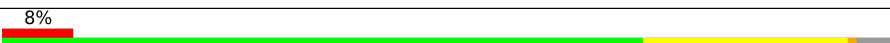
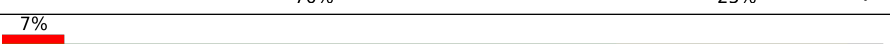
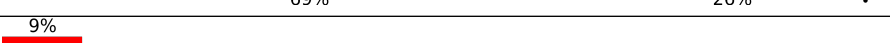
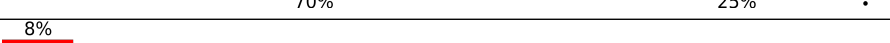
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10327 ( 2.20 - 3.20 )                                    |

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     | 548    |                  |
| 1   | B     | 548    |                  |
| 1   | C     | 548    |                  |
| 1   | D     | 548    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |     |
|-----|-------|--------|------------------------------------------------------------------------------------|-----|
| 1   | E     | 548    |  | • • |
| 1   | F     | 548    |  | • • |
| 1   | G     | 548    |  | • • |
| 1   | H     | 548    |  | • • |
| 1   | I     | 548    |  | •   |
| 1   | J     | 548    |  | • • |
| 1   | K     | 548    |  | •   |
| 1   | L     | 548    |  | •   |
| 1   | M     | 548    |  | •   |
| 1   | N     | 548    |  | • • |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 55646 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   | G     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | A     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | B     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | C     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | D     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | E     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | F     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | H     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | I     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | J     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | K     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | L     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | M     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |
| 1   | N     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3849  | 2392 | 665 | 772 | 20 |         |       |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 2   | A     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | B     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | C     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | D     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | E     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | F     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | H     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | I     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | J     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | K     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | L     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | M     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 2   | N     | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

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

| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 4   | G     | 1        | Total K<br>1 1 | 0       |
| 4   | A     | 1        | Total K<br>1 1 | 0       |
| 4   | B     | 1        | Total K<br>1 1 | 0       |
| 4   | C     | 1        | Total K<br>1 1 | 0       |
| 4   | D     | 1        | Total K<br>1 1 | 0       |
| 4   | E     | 1        | Total K<br>1 1 | 0       |
| 4   | F     | 1        | Total K<br>1 1 | 0       |
| 4   | H     | 1        | Total K<br>1 1 | 0       |
| 4   | I     | 1        | Total K<br>1 1 | 0       |
| 4   | J     | 1        | Total K<br>1 1 | 0       |
| 4   | K     | 1        | Total K<br>1 1 | 0       |
| 4   | L     | 1        | Total K<br>1 1 | 0       |
| 4   | M     | 1        | Total K<br>1 1 | 0       |
| 4   | N     | 1        | Total K<br>1 1 | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | AltConf |
|-----|-------|----------|--------------------|---------|
| 5   | G     | 92       | Total O<br>92 92   | 0       |
| 5   | A     | 101      | Total O<br>101 101 | 0       |
| 5   | B     | 99       | Total O<br>99 99   | 0       |
| 5   | C     | 102      | Total O<br>102 102 | 0       |
| 5   | D     | 89       | Total O<br>89 89   | 0       |

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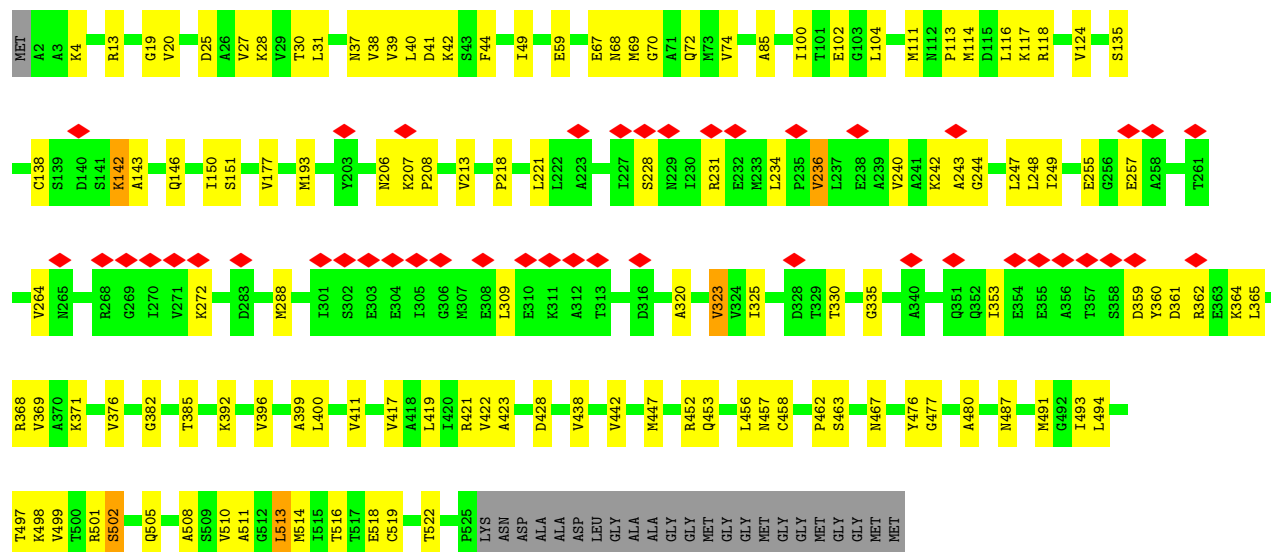
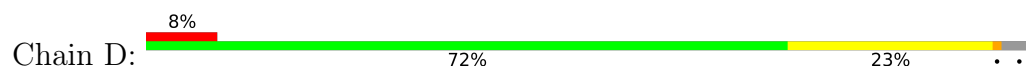
| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 5   | E     | 88       | Total<br>88  | O<br>88  | 0       |
| 5   | F     | 91       | Total<br>91  | O<br>91  | 0       |
| 5   | H     | 91       | Total<br>91  | O<br>91  | 0       |
| 5   | I     | 84       | Total<br>84  | O<br>84  | 0       |
| 5   | J     | 89       | Total<br>89  | O<br>89  | 0       |
| 5   | K     | 88       | Total<br>88  | O<br>88  | 0       |
| 5   | L     | 89       | Total<br>89  | O<br>89  | 0       |
| 5   | M     | 104      | Total<br>104 | O<br>104 | 0       |
| 5   | N     | 91       | Total<br>91  | O<br>91  | 0       |



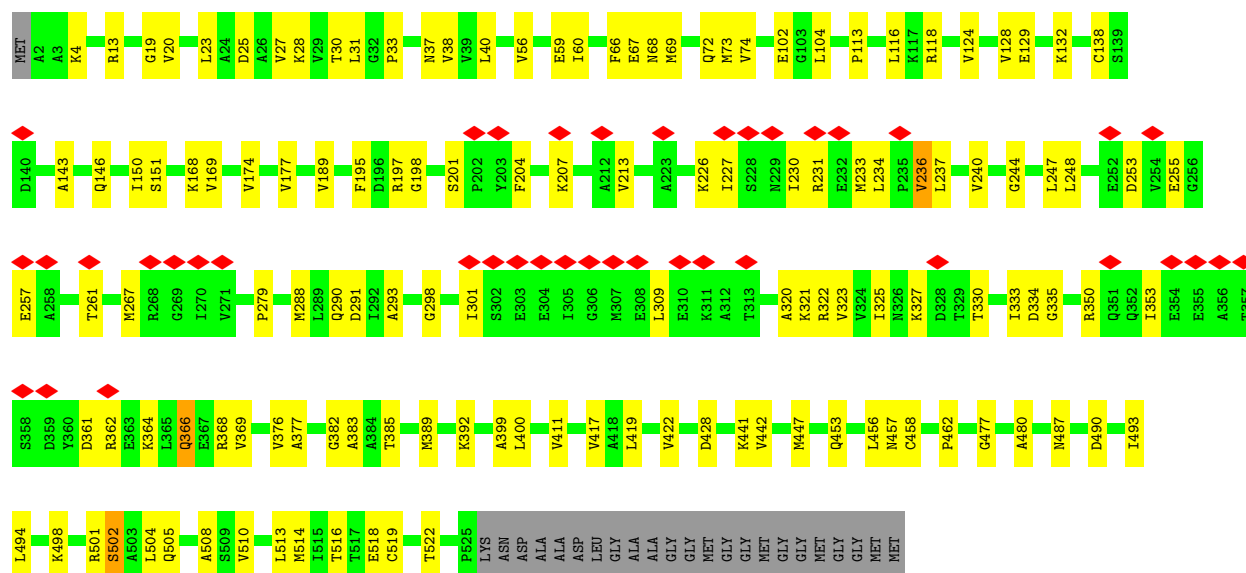


|      |
|------|
| P525 |
| LYS  |
| ASN  |
| ASP  |
| ALA  |
| ALA  |
| ASP  |
| LEU  |
| GLY  |
| ALA  |
| ALA  |
| GLY  |
| GLY  |
| MET  |
| GLY  |
| GLY  |
| MET  |
| GLY  |
| GLY  |
| MET  |
| MET  |

• Molecule 1: Chaperonin GroEL

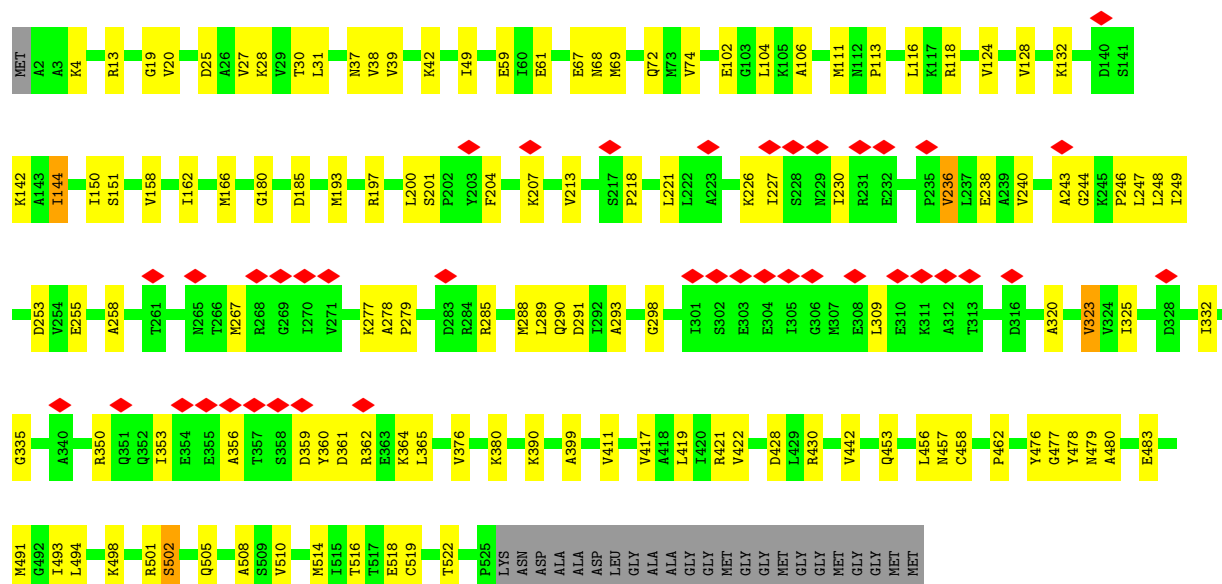


• Molecule 1: Chaperonin GroEL

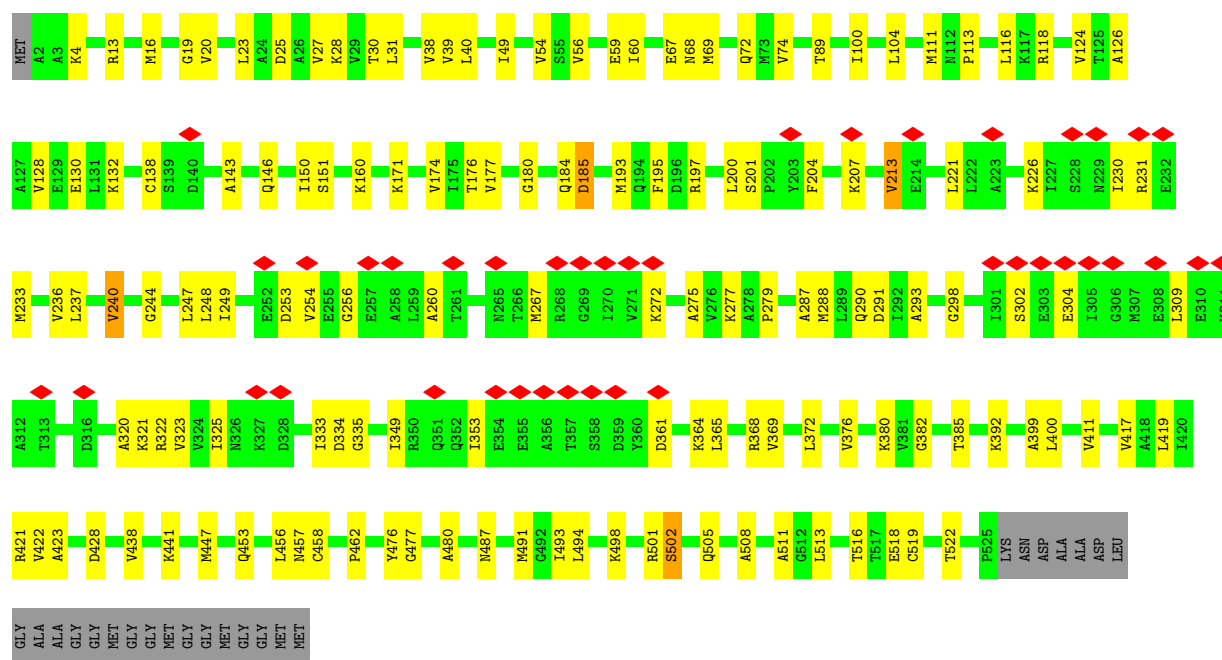


• Molecule 1: Chaperonin GroEL

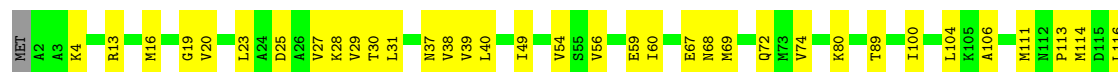


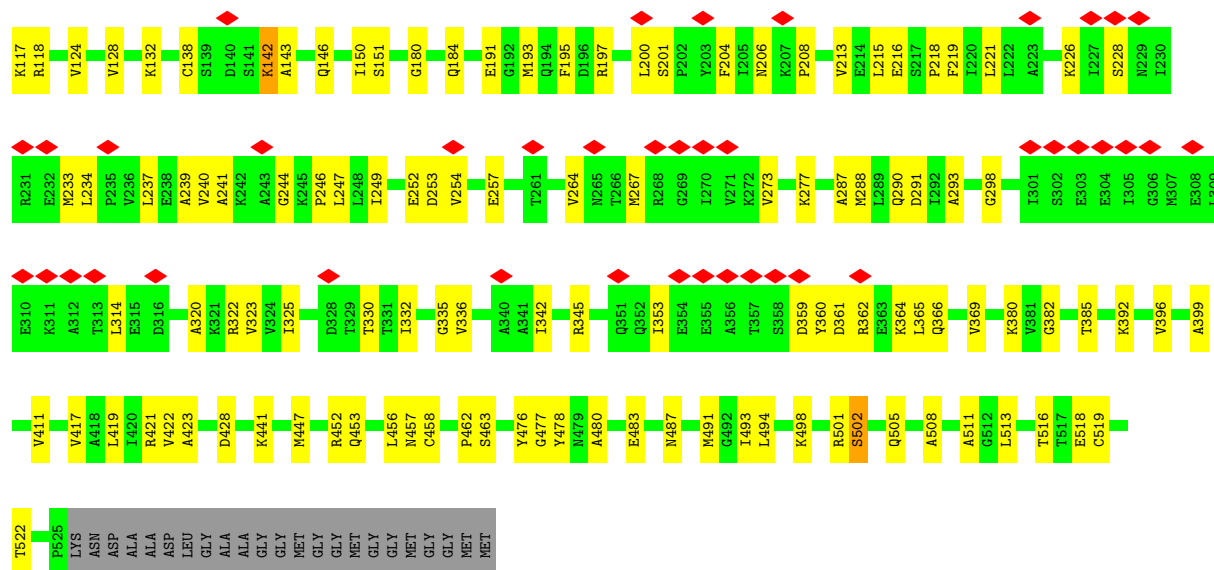


• Molecule 1: Chaperonin GroEL

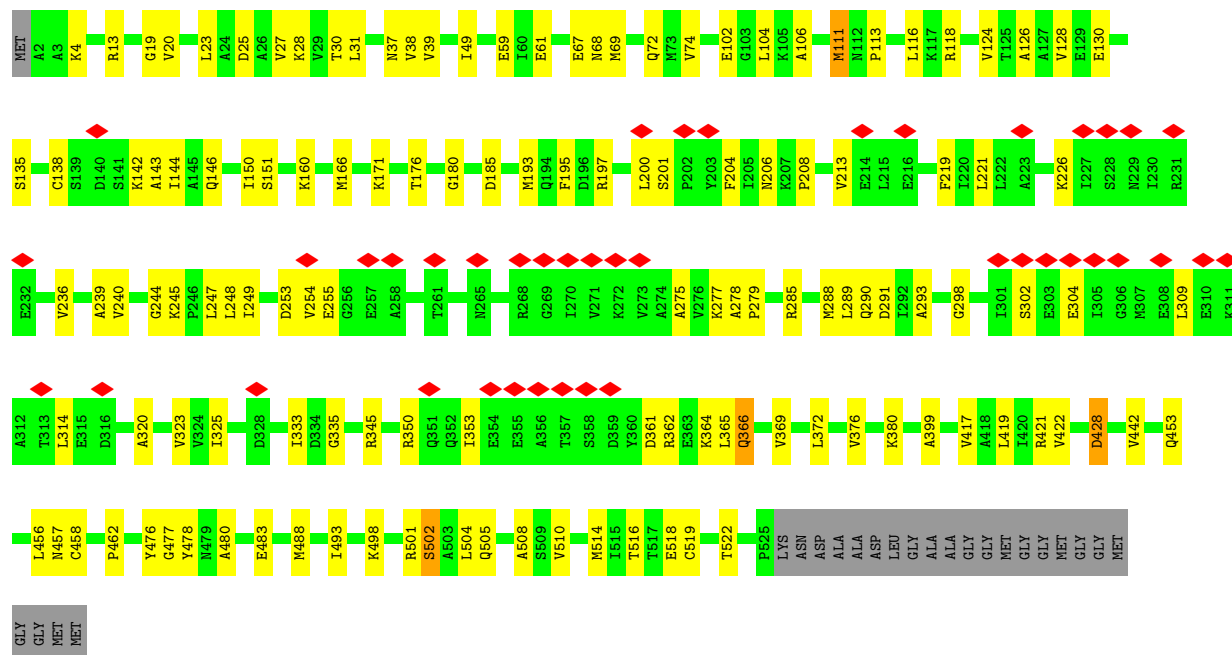


• Molecule 1: Chaperonin GroEL



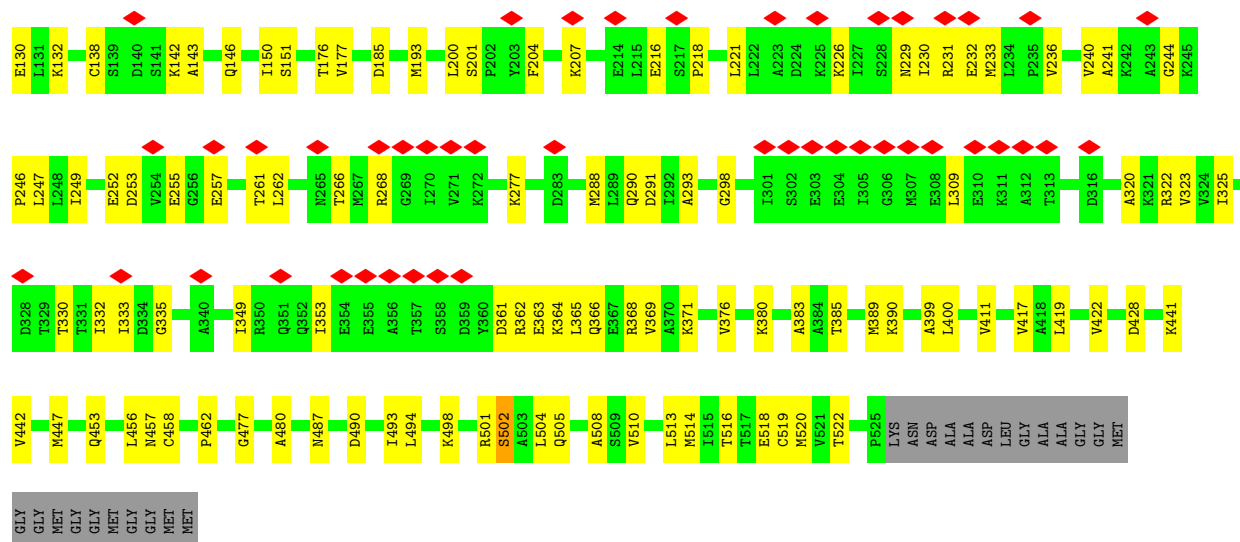


• Molecule 1: Chaperonin GroEL

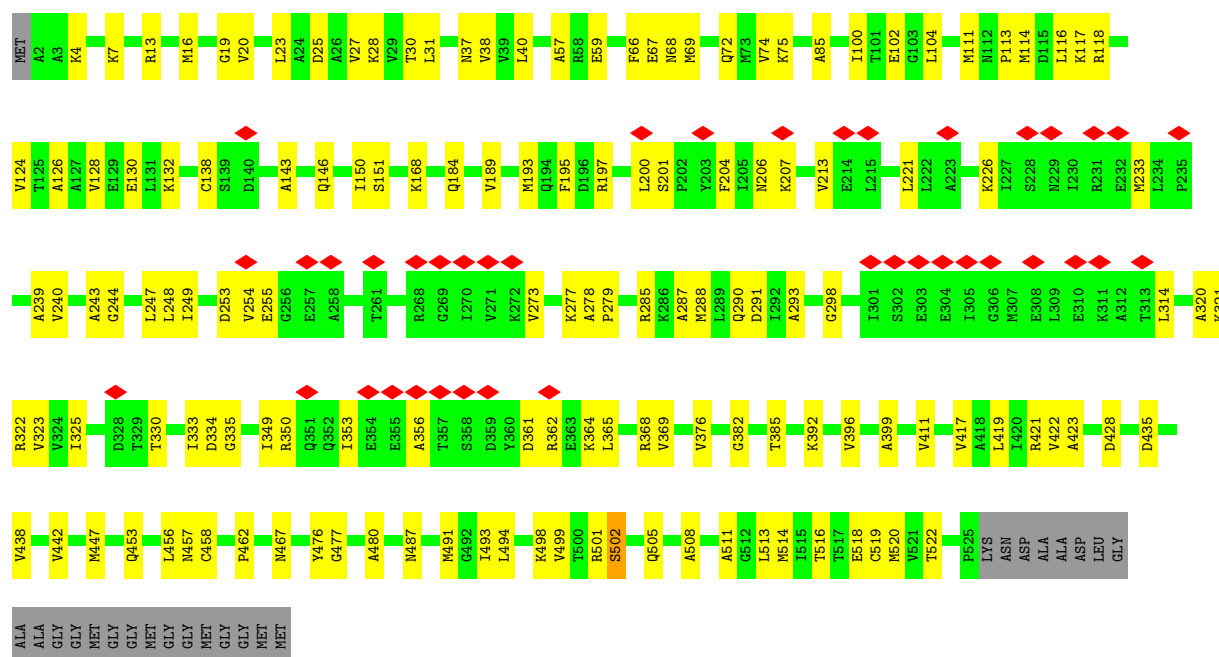


• Molecule 1: Chaperonin GroEL

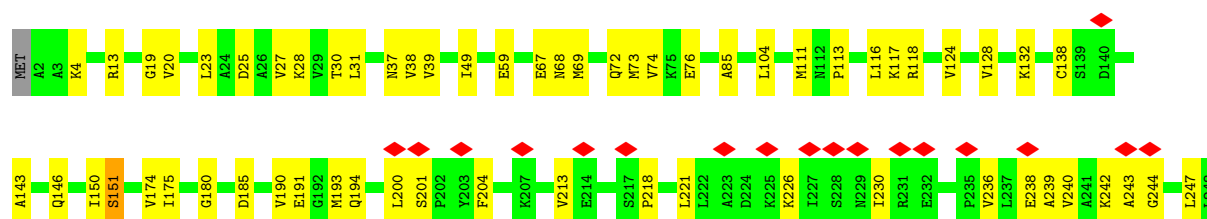


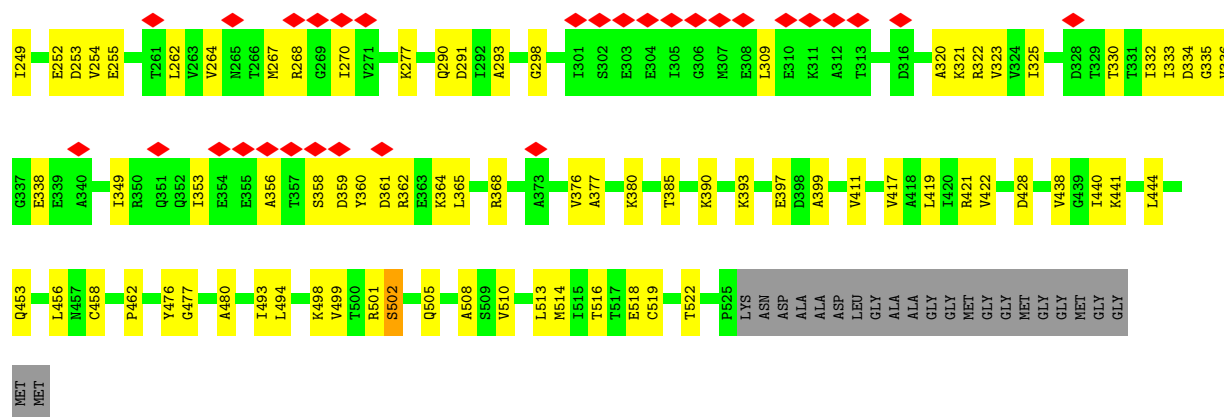


• Molecule 1: Chaperonin GroEL

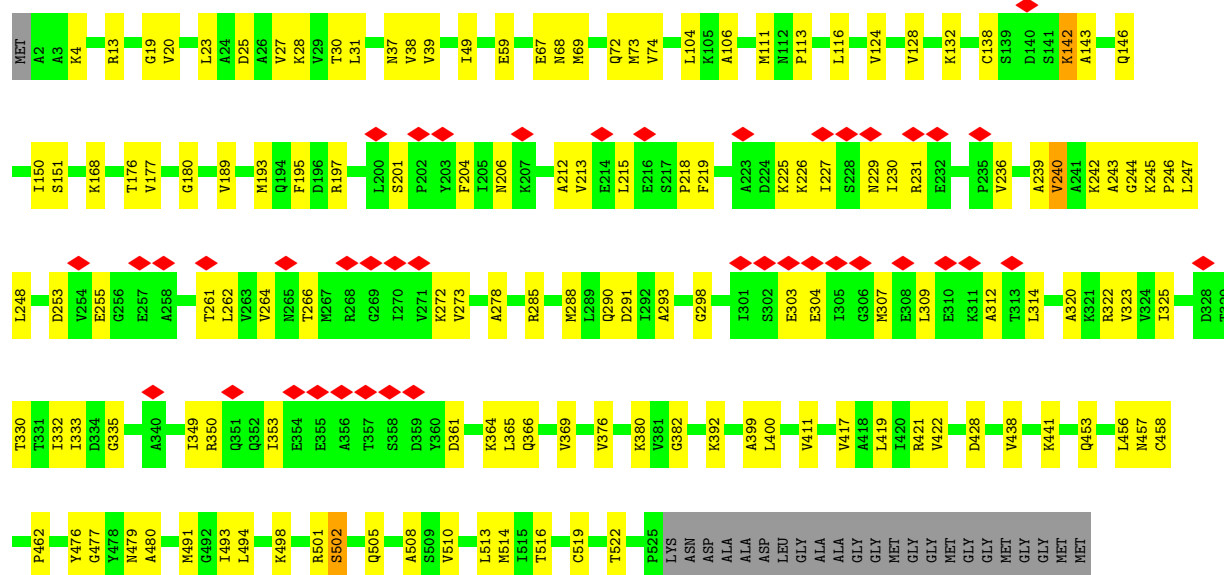


• Molecule 1: Chaperonin GroEL





### • Molecule 1: Chaperonin GroEL



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, D7                               | Depositor |
| Number of particles used             | 38440                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 63.6                                    | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | 60000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.282                                   | Depositor |
| Minimum map value                    | -0.090                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.019                                   | Depositor |
| Map size (Å)                         | 376.31998, 376.31998, 376.31998         | wwPDB     |
| Map dimensions                       | 392, 392, 392                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.9599999, 0.9599999, 0.9599999         | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.20         | 0/3876  | 0.28        | 0/5233  |
| 1   | B     | 0.20         | 0/3876  | 0.29        | 0/5233  |
| 1   | C     | 0.20         | 0/3876  | 0.30        | 0/5233  |
| 1   | D     | 0.20         | 0/3876  | 0.30        | 0/5233  |
| 1   | E     | 0.20         | 0/3876  | 0.29        | 0/5233  |
| 1   | F     | 0.20         | 0/3876  | 0.29        | 0/5233  |
| 1   | G     | 0.20         | 0/3876  | 0.29        | 0/5233  |
| 1   | H     | 0.20         | 0/3876  | 0.28        | 0/5233  |
| 1   | I     | 0.20         | 0/3876  | 0.31        | 0/5233  |
| 1   | J     | 0.20         | 0/3876  | 0.30        | 0/5233  |
| 1   | K     | 0.20         | 0/3876  | 0.28        | 0/5233  |
| 1   | L     | 0.20         | 0/3876  | 0.28        | 0/5233  |
| 1   | M     | 0.20         | 0/3876  | 0.30        | 0/5233  |
| 1   | N     | 0.20         | 0/3876  | 0.29        | 0/5233  |
| All | All   | 0.20         | 0/54264 | 0.29        | 0/73262 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | M     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | M     | 191 | GLU  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3849  | 0        | 3968     | 99      | 0            |
| 1   | B     | 3849  | 0        | 3968     | 87      | 0            |
| 1   | C     | 3849  | 0        | 3968     | 115     | 0            |
| 1   | D     | 3849  | 0        | 3967     | 100     | 0            |
| 1   | E     | 3849  | 0        | 3968     | 96      | 0            |
| 1   | F     | 3849  | 0        | 3967     | 93      | 0            |
| 1   | G     | 3849  | 0        | 3968     | 103     | 0            |
| 1   | H     | 3849  | 0        | 3968     | 99      | 0            |
| 1   | I     | 3849  | 0        | 3968     | 107     | 0            |
| 1   | J     | 3849  | 0        | 3967     | 89      | 0            |
| 1   | K     | 3849  | 0        | 3968     | 98      | 0            |
| 1   | L     | 3849  | 0        | 3968     | 101     | 0            |
| 1   | M     | 3849  | 0        | 3968     | 99      | 0            |
| 1   | N     | 3849  | 0        | 3968     | 97      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 31    | 0        | 12       | 0       | 0            |
| 3   | B     | 31    | 0        | 12       | 0       | 0            |
| 3   | C     | 31    | 0        | 12       | 1       | 0            |
| 3   | D     | 31    | 0        | 12       | 0       | 0            |
| 3   | E     | 31    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | F     | 31    | 0        | 12       | 0       | 0            |
| 3   | G     | 31    | 0        | 12       | 0       | 0            |
| 3   | H     | 31    | 0        | 12       | 0       | 0            |
| 3   | I     | 31    | 0        | 12       | 0       | 0            |
| 3   | J     | 31    | 0        | 12       | 0       | 0            |
| 3   | K     | 31    | 0        | 12       | 0       | 0            |
| 3   | L     | 31    | 0        | 12       | 0       | 0            |
| 3   | M     | 31    | 0        | 12       | 0       | 0            |
| 3   | N     | 31    | 0        | 12       | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 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     | 101   | 0        | 0        | 2       | 0            |
| 5   | B     | 99    | 0        | 0        | 3       | 0            |
| 5   | C     | 102   | 0        | 0        | 3       | 0            |
| 5   | D     | 89    | 0        | 0        | 2       | 0            |
| 5   | E     | 88    | 0        | 0        | 4       | 0            |
| 5   | F     | 91    | 0        | 0        | 2       | 0            |
| 5   | G     | 92    | 0        | 0        | 5       | 0            |
| 5   | H     | 91    | 0        | 0        | 2       | 0            |
| 5   | I     | 84    | 0        | 0        | 3       | 0            |
| 5   | J     | 89    | 0        | 0        | 2       | 0            |
| 5   | K     | 88    | 0        | 0        | 3       | 0            |
| 5   | L     | 89    | 0        | 0        | 2       | 0            |
| 5   | M     | 104   | 0        | 0        | 5       | 0            |
| 5   | N     | 91    | 0        | 0        | 1       | 0            |
| All | All   | 55646 | 0        | 55717    | 1262    | 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 11.

All (1262) 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:M:190:VAL:O    | 1:M:376:VAL:HB   | 1.69                     | 0.92              |
| 1:I:69:MET:HE2   | 1:I:522:THR:HB   | 1.58                     | 0.85              |
| 1:D:69:MET:HE2   | 1:D:522:THR:HB   | 1.58                     | 0.85              |
| 1:D:41:ASP:HB2   | 1:F:69:MET:HE2   | 1.59                     | 0.84              |
| 1:L:69:MET:HE2   | 1:L:522:THR:HB   | 1.60                     | 0.84              |
| 1:A:111:MET:HE3  | 1:A:438:VAL:HG11 | 1.61                     | 0.82              |
| 1:H:69:MET:HE2   | 1:H:522:THR:HB   | 1.62                     | 0.81              |
| 1:G:111:MET:HE3  | 1:G:438:VAL:HG11 | 1.62                     | 0.81              |
| 1:M:111:MET:HE3  | 1:M:438:VAL:HG11 | 1.61                     | 0.81              |
| 1:B:353:ILE:HG22 | 1:B:365:LEU:HB3  | 1.64                     | 0.80              |
| 1:D:193:MET:HE2  | 1:D:193:MET:HA   | 1.63                     | 0.79              |
| 1:N:353:ILE:HG22 | 1:N:365:LEU:HB3  | 1.65                     | 0.79              |
| 1:A:244:GLY:HA2  | 1:N:255:GLU:HG2  | 1.65                     | 0.78              |
| 1:C:263:VAL:HG22 | 1:C:267:MET:HE2  | 1.66                     | 0.77              |
| 1:J:69:MET:HE2   | 1:J:522:THR:HB   | 1.67                     | 0.76              |
| 1:H:353:ILE:HG12 | 1:H:365:LEU:HB3  | 1.69                     | 0.74              |
| 1:C:234:LEU:HA   | 1:C:237:LEU:HD12 | 1.69                     | 0.73              |
| 1:F:359:ASP:OD2  | 1:F:360:TYR:N    | 2.22                     | 0.73              |
| 1:D:359:ASP:OD2  | 1:D:360:TYR:N    | 2.22                     | 0.72              |
| 1:M:359:ASP:OD2  | 1:M:360:TYR:N    | 2.23                     | 0.71              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:HB2  | 1.71                     | 0.71              |
| 1:I:359:ASP:OD1  | 1:I:360:TYR:N    | 2.22                     | 0.71              |
| 1:A:349:ILE:O    | 1:A:353:ILE:HD12 | 1.92                     | 0.70              |
| 1:I:184:GLN:N    | 1:I:184:GLN:OE1  | 2.23                     | 0.70              |
| 1:D:240:VAL:HG11 | 1:D:247:LEU:HB2  | 1.73                     | 0.69              |
| 1:L:253:ASP:HB3  | 1:N:244:GLY:HA3  | 1.74                     | 0.69              |
| 1:E:288:MET:HE1  | 1:E:368:ARG:HG2  | 1.75                     | 0.69              |
| 1:I:353:ILE:HG12 | 1:I:365:LEU:HB3  | 1.75                     | 0.69              |
| 1:H:516:THR:OG1  | 1:J:37:ASN:ND2   | 2.25                     | 0.69              |
| 1:E:73:MET:HE3   | 1:E:514:MET:HE3  | 1.74                     | 0.68              |
| 1:E:69:MET:HE2   | 1:E:522:THR:HB   | 1.74                     | 0.68              |
| 1:K:73:MET:HE3   | 1:K:514:MET:HE3  | 1.75                     | 0.68              |
| 1:D:501:ARG:NH1  | 1:D:505:GLN:OE1  | 2.27                     | 0.68              |
| 1:I:336:VAL:O    | 5:I:701:HOH:O    | 2.12                     | 0.67              |
| 1:I:200:LEU:HD12 | 1:I:254:VAL:HG12 | 1.75                     | 0.67              |
| 1:L:501:ARG:NH1  | 1:L:505:GLN:OE1  | 2.28                     | 0.67              |
| 1:M:193:MET:HA   | 1:M:193:MET:HE2  | 1.77                     | 0.66              |
| 1:G:200:LEU:HD12 | 1:G:254:VAL:HG12 | 1.77                     | 0.66              |
| 1:A:117:LYS:NZ   | 5:A:704:HOH:O    | 2.28                     | 0.66              |
| 1:M:200:LEU:HD12 | 1:M:254:VAL:HG22 | 1.78                     | 0.66              |
| 1:C:501:ARG:NH1  | 1:C:505:GLN:OE1  | 2.29                     | 0.65              |
| 1:L:350:ARG:HA   | 1:L:353:ILE:HD12 | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:288:MET:HE1  | 1:G:368:ARG:HD2  | 1.79                     | 0.65              |
| 1:M:501:ARG:NH1  | 1:M:505:GLN:OE1  | 2.30                     | 0.65              |
| 1:N:236:VAL:HG21 | 1:N:309:LEU:HB3  | 1.79                     | 0.65              |
| 1:G:117:LYS:NZ   | 5:G:703:HOH:O    | 2.28                     | 0.65              |
| 1:A:69:MET:HE3   | 1:A:520:MET:HE2  | 1.78                     | 0.65              |
| 1:C:227:ILE:HD11 | 1:C:232:GLU:HB3  | 1.78                     | 0.65              |
| 1:D:74:VAL:HG13  | 1:D:514:MET:HE1  | 1.79                     | 0.65              |
| 1:I:226:LYS:HZ1  | 1:I:252:GLU:H    | 1.45                     | 0.65              |
| 1:F:240:VAL:HG11 | 1:F:247:LEU:HB2  | 1.79                     | 0.65              |
| 1:D:113:PRO:HB2  | 1:D:516:THR:HA   | 1.79                     | 0.65              |
| 1:B:365:LEU:HD23 | 1:B:368:ARG:HD3  | 1.78                     | 0.64              |
| 1:E:301:ILE:HD12 | 1:E:309:LEU:HG   | 1.79                     | 0.64              |
| 1:F:39:VAL:HG22  | 1:F:49:ILE:HG12  | 1.79                     | 0.64              |
| 1:K:323:VAL:HG12 | 1:K:332:ILE:HA   | 1.80                     | 0.64              |
| 1:H:213:VAL:HG22 | 1:H:325:ILE:HB   | 1.79                     | 0.64              |
| 1:G:69:MET:HE3   | 1:G:520:MET:HE2  | 1.79                     | 0.64              |
| 1:J:193:MET:HE1  | 1:J:195:PHE:HB3  | 1.79                     | 0.64              |
| 1:M:113:PRO:HB2  | 1:M:516:THR:HA   | 1.79                     | 0.64              |
| 1:H:287:ALA:HB3  | 1:H:288:MET:HE2  | 1.80                     | 0.64              |
| 1:G:69:MET:HE2   | 1:G:522:THR:HB   | 1.80                     | 0.64              |
| 1:M:117:LYS:NZ   | 5:M:708:HOH:O    | 2.31                     | 0.64              |
| 1:C:113:PRO:HB2  | 1:C:516:THR:HA   | 1.79                     | 0.63              |
| 1:L:20:VAL:HG21  | 1:L:514:MET:HE1  | 1.78                     | 0.63              |
| 1:H:501:ARG:NH1  | 1:H:505:GLN:OE1  | 2.31                     | 0.63              |
| 1:N:501:ARG:NH1  | 1:N:505:GLN:OE1  | 2.31                     | 0.63              |
| 1:A:193:MET:HE1  | 1:A:195:PHE:HB3  | 1.79                     | 0.63              |
| 1:E:501:ARG:NH1  | 1:E:505:GLN:OE1  | 2.32                     | 0.63              |
| 1:A:501:ARG:NH1  | 1:A:505:GLN:OE1  | 2.31                     | 0.63              |
| 1:B:501:ARG:NH1  | 1:B:505:GLN:OE1  | 2.32                     | 0.63              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:HB2  | 1.81                     | 0.63              |
| 1:G:353:ILE:HG12 | 1:G:365:LEU:HB3  | 1.80                     | 0.63              |
| 1:K:38:VAL:HG22  | 1:M:519:CYS:HB3  | 1.81                     | 0.63              |
| 1:N:143:ALA:HB1  | 1:N:146:GLN:HB2  | 1.80                     | 0.63              |
| 1:L:519:CYS:HB3  | 1:N:38:VAL:HG22  | 1.80                     | 0.62              |
| 1:C:23:LEU:HD22  | 1:C:74:VAL:HG13  | 1.81                     | 0.62              |
| 1:N:248:LEU:HD22 | 1:N:323:VAL:HG11 | 1.80                     | 0.62              |
| 1:J:69:MET:CE    | 1:J:522:THR:HB   | 2.27                     | 0.62              |
| 1:K:501:ARG:NH1  | 1:K:505:GLN:OE1  | 2.32                     | 0.62              |
| 1:I:501:ARG:NH1  | 1:I:505:GLN:OE1  | 2.33                     | 0.62              |
| 1:L:248:LEU:HD22 | 1:L:323:VAL:HG11 | 1.80                     | 0.62              |
| 1:C:519:CYS:HB3  | 1:E:38:VAL:HG22  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:510:VAL:HG12 | 1:D:514:MET:HE2  | 1.81                     | 0.62              |
| 1:D:20:VAL:HG13  | 1:D:74:VAL:HG11  | 1.80                     | 0.62              |
| 1:J:498:LYS:O    | 1:J:502:SER:OG   | 2.17                     | 0.62              |
| 1:C:248:LEU:HD22 | 1:C:323:VAL:HG11 | 1.79                     | 0.61              |
| 1:G:501:ARG:NH1  | 1:G:505:GLN:OE1  | 2.33                     | 0.61              |
| 1:C:193:MET:HE1  | 1:C:195:PHE:HB3  | 1.81                     | 0.61              |
| 1:D:288:MET:HE1  | 1:D:368:ARG:HD2  | 1.81                     | 0.61              |
| 1:F:498:LYS:O    | 1:F:502:SER:OG   | 2.18                     | 0.61              |
| 1:L:113:PRO:HB2  | 1:L:516:THR:HA   | 1.82                     | 0.61              |
| 1:E:248:LEU:HD22 | 1:E:323:VAL:HG11 | 1.82                     | 0.61              |
| 1:C:510:VAL:O    | 1:C:514:MET:HG3  | 2.00                     | 0.61              |
| 1:J:39:VAL:HG22  | 1:J:49:ILE:HG12  | 1.83                     | 0.61              |
| 1:K:365:LEU:HD23 | 1:K:368:ARG:HD3  | 1.81                     | 0.61              |
| 1:L:353:ILE:HD11 | 1:L:369:VAL:HG11 | 1.81                     | 0.61              |
| 1:A:234:LEU:O    | 1:A:238:GLU:HG2  | 2.01                     | 0.61              |
| 1:J:428:ASP:OD1  | 1:J:428:ASP:N    | 2.33                     | 0.61              |
| 1:K:113:PRO:HB2  | 1:K:516:THR:HA   | 1.83                     | 0.61              |
| 1:H:200:LEU:HD21 | 1:H:277:LYS:HG3  | 1.82                     | 0.61              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:HB2  | 1.81                     | 0.61              |
| 1:J:501:ARG:NH1  | 1:J:505:GLN:OE1  | 2.34                     | 0.61              |
| 1:A:248:LEU:HD22 | 1:A:323:VAL:HG11 | 1.82                     | 0.60              |
| 1:B:38:VAL:HG22  | 1:D:519:CYS:HB3  | 1.83                     | 0.60              |
| 1:G:20:VAL:HG13  | 1:G:74:VAL:HG21  | 1.83                     | 0.60              |
| 1:F:353:ILE:O    | 1:F:362:ARG:NH2  | 2.33                     | 0.60              |
| 1:H:193:MET:HE1  | 1:H:195:PHE:HB3  | 1.82                     | 0.60              |
| 1:N:498:LYS:O    | 1:N:502:SER:OG   | 2.15                     | 0.60              |
| 1:L:255:GLU:OE2  | 1:N:243:ALA:N    | 2.34                     | 0.60              |
| 1:F:428:ASP:OD1  | 1:F:428:ASP:N    | 2.34                     | 0.60              |
| 1:G:242:LYS:HG3  | 1:B:226:LYS:HE3  | 1.83                     | 0.60              |
| 1:L:23:LEU:HD22  | 1:L:74:VAL:HG13  | 1.83                     | 0.60              |
| 1:L:143:ALA:HB1  | 1:L:146:GLN:HB2  | 1.83                     | 0.60              |
| 1:G:519:CYS:HB3  | 1:M:38:VAL:HG22  | 1.84                     | 0.60              |
| 1:F:501:ARG:NH1  | 1:F:505:GLN:OE1  | 2.35                     | 0.60              |
| 1:H:248:LEU:HD22 | 1:H:323:VAL:HG11 | 1.83                     | 0.60              |
| 1:H:253:ASP:HB3  | 1:J:244:GLY:HA3  | 1.83                     | 0.60              |
| 1:N:20:VAL:HG13  | 1:N:74:VAL:HG21  | 1.82                     | 0.60              |
| 1:G:336:VAL:O    | 5:G:701:HOH:O    | 2.17                     | 0.60              |
| 1:A:20:VAL:HG13  | 1:A:74:VAL:HG21  | 1.84                     | 0.60              |
| 1:B:498:LYS:O    | 1:B:502:SER:OG   | 2.15                     | 0.60              |
| 1:M:510:VAL:O    | 1:M:514:MET:HG3  | 2.02                     | 0.60              |
| 1:A:38:VAL:HG22  | 1:N:519:CYS:HB3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:69:MET:HE2   | 1:A:522:THR:HB   | 1.84                     | 0.60              |
| 1:M:458:CYS:SG   | 1:M:480:ALA:HB1  | 2.42                     | 0.60              |
| 1:C:365:LEU:HD23 | 1:C:368:ARG:HD3  | 1.82                     | 0.60              |
| 1:F:38:VAL:HG22  | 1:I:519:CYS:HB3  | 1.82                     | 0.60              |
| 1:I:20:VAL:HG13  | 1:I:74:VAL:HG21  | 1.83                     | 0.60              |
| 1:N:69:MET:O     | 1:N:73:MET:HG3   | 2.01                     | 0.60              |
| 1:H:498:LYS:O    | 1:H:502:SER:OG   | 2.16                     | 0.59              |
| 1:B:113:PRO:HB2  | 1:B:516:THR:HA   | 1.84                     | 0.59              |
| 1:H:20:VAL:HG13  | 1:H:74:VAL:HG21  | 1.83                     | 0.59              |
| 1:I:498:LYS:O    | 1:I:502:SER:OG   | 2.16                     | 0.59              |
| 1:M:353:ILE:HG12 | 1:M:365:LEU:HB3  | 1.84                     | 0.59              |
| 1:K:20:VAL:HG13  | 1:K:74:VAL:HG21  | 1.83                     | 0.59              |
| 1:L:193:MET:HE1  | 1:L:195:PHE:HB3  | 1.84                     | 0.59              |
| 1:E:290:GLN:NE2  | 1:E:291:ASP:OD1  | 2.36                     | 0.59              |
| 1:F:113:PRO:HB2  | 1:F:516:THR:HA   | 1.85                     | 0.59              |
| 1:I:38:VAL:HG22  | 1:K:519:CYS:HB3  | 1.85                     | 0.59              |
| 1:J:248:LEU:HD22 | 1:J:323:VAL:HG11 | 1.84                     | 0.59              |
| 1:E:23:LEU:HD22  | 1:E:74:VAL:HG12  | 1.84                     | 0.59              |
| 1:F:69:MET:CE    | 1:F:522:THR:HB   | 2.32                     | 0.59              |
| 1:J:20:VAL:HG13  | 1:J:74:VAL:HG21  | 1.83                     | 0.59              |
| 1:N:73:MET:HE3   | 1:N:514:MET:HE3  | 1.85                     | 0.59              |
| 1:A:113:PRO:HB2  | 1:A:516:THR:HA   | 1.85                     | 0.59              |
| 1:C:458:CYS:SG   | 1:C:480:ALA:HB1  | 2.43                     | 0.59              |
| 1:G:13:ARG:NH1   | 1:G:518:GLU:OE1  | 2.30                     | 0.59              |
| 1:L:57:ALA:O     | 1:L:75:LYS:HE2   | 2.01                     | 0.59              |
| 1:G:113:PRO:HB2  | 1:G:516:THR:HA   | 1.85                     | 0.58              |
| 1:H:39:VAL:HG22  | 1:H:49:ILE:HG12  | 1.85                     | 0.58              |
| 1:I:323:VAL:HG12 | 1:I:332:ILE:HA   | 1.84                     | 0.58              |
| 1:L:200:LEU:HD21 | 1:L:277:LYS:HG3  | 1.85                     | 0.58              |
| 1:G:365:LEU:HD23 | 1:G:368:ARG:HD3  | 1.85                     | 0.58              |
| 1:F:20:VAL:HG13  | 1:F:74:VAL:HG21  | 1.85                     | 0.58              |
| 1:F:288:MET:SD   | 1:F:289:LEU:N    | 2.76                     | 0.58              |
| 1:G:458:CYS:SG   | 1:G:480:ALA:HB1  | 2.44                     | 0.58              |
| 1:J:113:PRO:HB2  | 1:J:516:THR:HA   | 1.86                     | 0.58              |
| 1:M:353:ILE:HA   | 1:M:362:ARG:NH2  | 2.18                     | 0.58              |
| 1:B:20:VAL:HG13  | 1:B:74:VAL:HG21  | 1.84                     | 0.58              |
| 1:E:234:LEU:HA   | 1:E:237:LEU:HD12 | 1.85                     | 0.58              |
| 1:F:69:MET:HE1   | 1:F:522:THR:HB   | 1.84                     | 0.58              |
| 1:C:213:VAL:HG22 | 1:C:325:ILE:HB   | 1.85                     | 0.58              |
| 1:D:423:ALA:HB2  | 1:D:447:MET:HE2  | 1.84                     | 0.58              |
| 1:E:124:VAL:HG21 | 1:E:508:ALA:HB2  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:510:VAL:O    | 1:J:514:MET:HG3  | 2.04                     | 0.58              |
| 1:F:197:ARG:HG3  | 1:F:279:PRO:HD3  | 1.84                     | 0.58              |
| 1:F:510:VAL:O    | 1:F:514:MET:HG3  | 2.04                     | 0.58              |
| 1:J:488:MET:HE2  | 1:J:488:MET:HA   | 1.84                     | 0.58              |
| 1:M:151:SER:HB2  | 1:M:399:ALA:HA   | 1.84                     | 0.58              |
| 1:D:38:VAL:HG22  | 1:F:519:CYS:HB3  | 1.84                     | 0.58              |
| 1:D:39:VAL:HG22  | 1:D:49:ILE:HG12  | 1.84                     | 0.58              |
| 1:F:213:VAL:HG22 | 1:F:325:ILE:HB   | 1.85                     | 0.58              |
| 1:L:184:GLN:N    | 1:L:184:GLN:OE1  | 2.37                     | 0.58              |
| 1:N:113:PRO:HB2  | 1:N:516:THR:HA   | 1.86                     | 0.58              |
| 1:D:458:CYS:SG   | 1:D:480:ALA:HB1  | 2.44                     | 0.58              |
| 1:E:20:VAL:HG13  | 1:E:74:VAL:HG21  | 1.85                     | 0.58              |
| 1:E:519:CYS:HB3  | 1:H:38:VAL:HG22  | 1.86                     | 0.58              |
| 1:L:423:ALA:HB2  | 1:L:447:MET:HE2  | 1.84                     | 0.58              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:HB2  | 1.85                     | 0.58              |
| 1:H:184:GLN:OE1  | 1:H:184:GLN:N    | 2.37                     | 0.57              |
| 1:K:23:LEU:HD22  | 1:K:74:VAL:HG12  | 1.86                     | 0.57              |
| 1:L:365:LEU:HD23 | 1:L:368:ARG:HD3  | 1.86                     | 0.57              |
| 1:A:458:CYS:SG   | 1:A:480:ALA:HB1  | 2.44                     | 0.57              |
| 1:L:458:CYS:SG   | 1:L:480:ALA:HB1  | 2.44                     | 0.57              |
| 1:A:118:ARG:NH2  | 5:A:712:HOH:O    | 2.36                     | 0.57              |
| 1:B:458:CYS:SG   | 1:B:480:ALA:HB1  | 2.44                     | 0.57              |
| 1:H:519:CYS:HB3  | 1:J:38:VAL:HG22  | 1.85                     | 0.57              |
| 1:K:124:VAL:HG21 | 1:K:508:ALA:HB2  | 1.85                     | 0.57              |
| 1:L:255:GLU:OE2  | 1:N:244:GLY:N    | 2.32                     | 0.57              |
| 1:E:353:ILE:HA   | 1:E:362:ARG:NH2  | 2.19                     | 0.57              |
| 1:K:200:LEU:HD21 | 1:K:277:LYS:HG3  | 1.85                     | 0.57              |
| 1:M:20:VAL:HG13  | 1:M:74:VAL:HG21  | 1.87                     | 0.57              |
| 1:N:193:MET:HE1  | 1:N:195:PHE:HB3  | 1.86                     | 0.57              |
| 1:I:226:LYS:HE3  | 1:I:252:GLU:HB3  | 1.86                     | 0.57              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:A:13:ARG:NH1   | 1:A:518:GLU:OE1  | 2.31                     | 0.57              |
| 1:F:278:ALA:HB3  | 1:F:285:ARG:HH11 | 1.68                     | 0.57              |
| 1:F:458:CYS:SG   | 1:F:480:ALA:HB1  | 2.44                     | 0.57              |
| 1:I:428:ASP:OD1  | 1:I:428:ASP:N    | 2.36                     | 0.57              |
| 1:L:498:LYS:O    | 1:L:502:SER:OG   | 2.16                     | 0.57              |
| 1:N:229:ASN:OD1  | 1:N:231:ARG:N    | 2.36                     | 0.57              |
| 1:H:428:ASP:OD1  | 1:H:428:ASP:N    | 2.35                     | 0.57              |
| 1:J:350:ARG:HA   | 1:J:353:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:247:LEU:HB3  | 1:A:273:VAL:HG22 | 1.86                     | 0.57              |
| 1:A:519:CYS:HB3  | 1:C:38:VAL:HG22  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:197:ARG:HD2  | 1:B:277:LYS:HB2  | 1.87                     | 0.57              |
| 1:E:458:CYS:SG   | 1:E:480:ALA:HB1  | 2.45                     | 0.57              |
| 1:N:458:CYS:SG   | 1:N:480:ALA:HB1  | 2.45                     | 0.57              |
| 1:G:38:VAL:HG22  | 1:B:519:CYS:HB3  | 1.86                     | 0.56              |
| 1:E:213:VAL:HG22 | 1:E:325:ILE:HB   | 1.86                     | 0.56              |
| 1:G:421:ARG:NH2  | 1:G:476:TYR:O    | 2.37                     | 0.56              |
| 1:A:242:LYS:HD3  | 1:N:227:ILE:HG13 | 1.87                     | 0.56              |
| 1:N:111:MET:HE1  | 1:N:438:VAL:HG21 | 1.87                     | 0.56              |
| 1:G:27:VAL:O     | 1:G:30:THR:OG1   | 2.15                     | 0.56              |
| 1:D:353:ILE:HG12 | 1:D:365:LEU:HB3  | 1.87                     | 0.56              |
| 1:D:498:LYS:O    | 1:D:502:SER:OG   | 2.17                     | 0.56              |
| 1:E:498:LYS:O    | 1:E:502:SER:OG   | 2.17                     | 0.56              |
| 1:H:254:VAL:HG21 | 1:H:275:ALA:HB1  | 1.86                     | 0.56              |
| 1:H:458:CYS:SG   | 1:H:480:ALA:HB1  | 2.45                     | 0.56              |
| 1:K:320:ALA:HA   | 1:K:335:GLY:HA2  | 1.87                     | 0.56              |
| 1:K:458:CYS:SG   | 1:K:480:ALA:HB1  | 2.45                     | 0.56              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HD22 | 1.87                     | 0.56              |
| 1:D:118:ARG:NH2  | 5:D:711:HOH:O    | 2.36                     | 0.56              |
| 1:E:236:VAL:HG21 | 1:E:309:LEU:HB3  | 1.87                     | 0.56              |
| 1:E:257:GLU:HA   | 1:H:267:MET:HB3  | 1.88                     | 0.56              |
| 1:I:234:LEU:HA   | 1:I:237:LEU:HD12 | 1.88                     | 0.56              |
| 1:K:69:MET:HE2   | 1:K:522:THR:HB   | 1.87                     | 0.56              |
| 1:A:244:GLY:H    | 1:N:253:ASP:HB3  | 1.71                     | 0.56              |
| 1:G:118:ARG:NH2  | 5:G:709:HOH:O    | 2.35                     | 0.56              |
| 1:C:353:ILE:HG12 | 1:C:365:LEU:HB3  | 1.88                     | 0.56              |
| 1:I:191:GLU:HG2  | 1:I:342:ILE:HD13 | 1.85                     | 0.56              |
| 1:B:349:ILE:O    | 1:B:353:ILE:HG23 | 2.06                     | 0.56              |
| 1:E:113:PRO:HB2  | 1:E:516:THR:HA   | 1.88                     | 0.56              |
| 1:I:458:CYS:SG   | 1:I:480:ALA:HB1  | 2.45                     | 0.56              |
| 1:J:458:CYS:SG   | 1:J:480:ALA:HB1  | 2.46                     | 0.56              |
| 1:L:287:ALA:HB3  | 1:L:288:MET:HE2  | 1.86                     | 0.56              |
| 1:M:236:VAL:HG21 | 1:M:309:LEU:HB3  | 1.86                     | 0.56              |
| 1:G:320:ALA:HA   | 1:G:335:GLY:HA2  | 1.88                     | 0.56              |
| 1:A:361:ASP:HA   | 1:A:364:LYS:HG2  | 1.88                     | 0.56              |
| 1:B:143:ALA:HB1  | 1:B:146:GLN:HB2  | 1.88                     | 0.56              |
| 1:K:498:LYS:O    | 1:K:502:SER:OG   | 2.17                     | 0.56              |
| 1:A:358:SER:O    | 1:A:362:ARG:N    | 2.35                     | 0.56              |
| 1:C:31:LEU:HD23  | 1:C:453:GLN:HB3  | 1.88                     | 0.56              |
| 1:D:213:VAL:HG22 | 1:D:325:ILE:HB   | 1.88                     | 0.56              |
| 1:E:66:PHE:HA    | 1:E:69:MET:HE3   | 1.87                     | 0.56              |
| 1:I:40:LEU:HD13  | 1:I:59:GLU:HG3   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:290:GLN:NE2  | 1:N:291:ASP:OD1  | 2.38                     | 0.56              |
| 1:D:13:ARG:NH1   | 1:D:518:GLU:OE1  | 2.34                     | 0.55              |
| 1:L:118:ARG:NH2  | 5:L:711:HOH:O    | 2.37                     | 0.55              |
| 1:M:322:ARG:HG2  | 1:M:333:ILE:HD12 | 1.86                     | 0.55              |
| 1:B:271:VAL:HG21 | 1:D:255:GLU:HG2  | 1.89                     | 0.55              |
| 1:H:382:GLY:O    | 1:H:392:LYS:NZ   | 2.36                     | 0.55              |
| 1:A:23:LEU:HD22  | 1:A:74:VAL:HG12  | 1.88                     | 0.55              |
| 1:C:253:ASP:HB3  | 1:E:244:GLY:HA3  | 1.89                     | 0.55              |
| 1:A:498:LYS:O    | 1:A:502:SER:OG   | 2.16                     | 0.55              |
| 1:E:13:ARG:NH1   | 1:E:518:GLU:OE1  | 2.33                     | 0.55              |
| 1:H:423:ALA:HB2  | 1:H:447:MET:HE2  | 1.87                     | 0.55              |
| 1:D:365:LEU:HD23 | 1:D:368:ARG:HD3  | 1.88                     | 0.55              |
| 1:M:336:VAL:O    | 5:M:701:HOH:O    | 2.18                     | 0.55              |
| 1:E:143:ALA:HB1  | 1:E:146:GLN:HB2  | 1.88                     | 0.55              |
| 1:I:113:PRO:HB2  | 1:I:516:THR:HA   | 1.89                     | 0.55              |
| 1:L:362:ARG:HH12 | 1:L:365:LEU:HD12 | 1.72                     | 0.55              |
| 1:M:213:VAL:HG22 | 1:M:325:ILE:HB   | 1.89                     | 0.55              |
| 1:B:243:ALA:O    | 1:D:255:GLU:N    | 2.40                     | 0.55              |
| 1:N:23:LEU:HD22  | 1:N:74:VAL:HG12  | 1.88                     | 0.55              |
| 1:G:498:LYS:O    | 1:G:502:SER:OG   | 2.16                     | 0.55              |
| 1:B:366:GLN:HA   | 1:B:369:VAL:HG22 | 1.89                     | 0.55              |
| 1:D:242:LYS:NZ   | 1:F:227:ILE:O    | 2.37                     | 0.55              |
| 1:E:129:GLU:OE1  | 5:E:701:HOH:O    | 2.17                     | 0.55              |
| 1:E:195:PHE:HB2  | 1:E:279:PRO:HG3  | 1.89                     | 0.54              |
| 1:F:13:ARG:NH1   | 1:F:518:GLU:OE1  | 2.35                     | 0.54              |
| 1:F:236:VAL:HG21 | 1:F:309:LEU:HB3  | 1.89                     | 0.54              |
| 1:C:516:THR:OG1  | 1:E:37:ASN:ND2   | 2.37                     | 0.54              |
| 1:C:229:ASN:OD1  | 1:C:232:GLU:N    | 2.39                     | 0.54              |
| 1:D:243:ALA:HA   | 1:F:226:LYS:HD2  | 1.88                     | 0.54              |
| 1:E:361:ASP:HA   | 1:E:364:LYS:HG2  | 1.89                     | 0.54              |
| 1:I:320:ALA:HA   | 1:I:335:GLY:HA2  | 1.88                     | 0.54              |
| 1:J:302:SER:OG   | 1:J:304:GLU:OE1  | 2.25                     | 0.54              |
| 1:A:255:GLU:HB3  | 1:C:271:VAL:HG21 | 1.88                     | 0.54              |
| 1:H:113:PRO:HB2  | 1:H:516:THR:HA   | 1.90                     | 0.54              |
| 1:D:221:LEU:HD23 | 1:D:249:ILE:HG12 | 1.88                     | 0.54              |
| 1:I:39:VAL:HG22  | 1:I:49:ILE:HG12  | 1.88                     | 0.54              |
| 1:M:361:ASP:HA   | 1:M:364:LYS:HG2  | 1.89                     | 0.54              |
| 1:C:498:LYS:O    | 1:C:502:SER:OG   | 2.17                     | 0.54              |
| 1:K:143:ALA:HB1  | 1:K:146:GLN:HB2  | 1.89                     | 0.54              |
| 1:G:247:LEU:HB3  | 1:G:273:VAL:HG22 | 1.88                     | 0.54              |
| 1:B:267:MET:HB3  | 1:D:257:GLU:HA   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:126:ALA:O    | 1:J:130:GLU:HG2  | 2.08                     | 0.54              |
| 1:D:421:ARG:NH2  | 1:D:476:TYR:O    | 2.40                     | 0.53              |
| 1:C:428:ASP:OD1  | 1:C:428:ASP:N    | 2.41                     | 0.53              |
| 1:E:428:ASP:OD1  | 1:E:428:ASP:N    | 2.38                     | 0.53              |
| 1:G:105:LYS:NZ   | 5:G:710:HOH:O    | 2.36                     | 0.53              |
| 1:A:253:ASP:HB3  | 1:C:244:GLY:HA3  | 1.91                     | 0.53              |
| 1:C:124:VAL:HG21 | 1:C:508:ALA:HB2  | 1.89                     | 0.53              |
| 1:E:382:GLY:O    | 1:E:392:LYS:NZ   | 2.37                     | 0.53              |
| 1:K:13:ARG:NH1   | 1:K:518:GLU:OE1  | 2.35                     | 0.53              |
| 1:M:498:LYS:O    | 1:M:502:SER:OG   | 2.17                     | 0.53              |
| 1:A:421:ARG:NH2  | 1:A:476:TYR:O    | 2.40                     | 0.53              |
| 1:M:320:ALA:HA   | 1:M:335:GLY:HA2  | 1.90                     | 0.53              |
| 1:C:176:THR:HG21 | 1:C:333:ILE:HD11 | 1.91                     | 0.53              |
| 1:H:40:LEU:HD13  | 1:H:59:GLU:HG3   | 1.90                     | 0.53              |
| 1:J:519:CYS:HB3  | 1:L:38:VAL:HG22  | 1.89                     | 0.53              |
| 1:K:226:LYS:HD3  | 1:K:252:GLU:HB3  | 1.91                     | 0.53              |
| 1:M:31:LEU:HD23  | 1:M:453:GLN:HB3  | 1.89                     | 0.53              |
| 1:M:393:LYS:NZ   | 1:M:397:GLU:OE2  | 2.41                     | 0.53              |
| 1:H:124:VAL:HG21 | 1:H:508:ALA:HB2  | 1.90                     | 0.53              |
| 1:I:124:VAL:HG21 | 1:I:508:ALA:HB2  | 1.90                     | 0.53              |
| 1:M:124:VAL:HG21 | 1:M:508:ALA:HB2  | 1.90                     | 0.53              |
| 1:M:428:ASP:OD1  | 1:M:428:ASP:N    | 2.41                     | 0.53              |
| 1:G:226:LYS:HD2  | 1:M:243:ALA:HA   | 1.90                     | 0.53              |
| 1:C:25:ASP:HA    | 1:C:28:LYS:HG2   | 1.91                     | 0.53              |
| 1:N:106:ALA:O    | 1:N:111:MET:HG3  | 2.07                     | 0.53              |
| 1:G:221:LEU:HD23 | 1:G:249:ILE:HG12 | 1.89                     | 0.53              |
| 1:H:207:LYS:NZ   | 5:H:711:HOH:O    | 2.35                     | 0.53              |
| 1:M:25:ASP:HA    | 1:M:28:LYS:HG2   | 1.91                     | 0.53              |
| 1:N:68:ASN:O     | 1:N:72:GLN:HG2   | 2.08                     | 0.53              |
| 1:A:143:ALA:HB1  | 1:A:146:GLN:HB2  | 1.90                     | 0.53              |
| 1:I:213:VAL:HG12 | 1:I:325:ILE:HB   | 1.90                     | 0.53              |
| 1:I:361:ASP:HA   | 1:I:364:LYS:HE3  | 1.91                     | 0.53              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:HB2  | 1.91                     | 0.53              |
| 1:K:37:ASN:ND2   | 1:M:516:THR:OG1  | 2.39                     | 0.53              |
| 1:G:37:ASN:ND2   | 1:B:516:THR:OG1  | 2.35                     | 0.52              |
| 1:I:221:LEU:HD23 | 1:I:249:ILE:HG12 | 1.91                     | 0.52              |
| 1:C:236:VAL:HG21 | 1:C:309:LEU:HB3  | 1.92                     | 0.52              |
| 1:C:320:ALA:HA   | 1:C:335:GLY:HA2  | 1.91                     | 0.52              |
| 1:E:13:ARG:HD2   | 1:E:104:LEU:HD22 | 1.91                     | 0.52              |
| 1:F:350:ARG:HA   | 1:F:353:ILE:HD12 | 1.92                     | 0.52              |
| 1:H:143:ALA:HB1  | 1:H:146:GLN:HB2  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:195:PHE:CD2  | 1:E:197:ARG:HB2  | 2.43                     | 0.52              |
| 1:I:423:ALA:HB2  | 1:I:447:MET:HE2  | 1.91                     | 0.52              |
| 1:K:25:ASP:HA    | 1:K:28:LYS:HG2   | 1.92                     | 0.52              |
| 1:C:33:PRO:HG3   | 3:C:602:ATP:C5   | 2.44                     | 0.52              |
| 1:F:124:VAL:HG21 | 1:F:508:ALA:HB2  | 1.91                     | 0.52              |
| 1:F:144:ILE:HG21 | 1:F:166:MET:SD   | 2.49                     | 0.52              |
| 1:I:118:ARG:NH2  | 5:I:711:HOH:O    | 2.43                     | 0.52              |
| 1:I:233:MET:SD   | 1:I:237:LEU:HG   | 2.49                     | 0.52              |
| 1:J:226:LYS:HD2  | 1:L:243:ALA:HA   | 1.91                     | 0.52              |
| 1:G:23:LEU:HD22  | 1:G:74:VAL:HG12  | 1.90                     | 0.52              |
| 1:F:37:ASN:ND2   | 1:I:516:THR:OG1  | 2.38                     | 0.52              |
| 1:G:240:VAL:HG21 | 1:G:247:LEU:HB2  | 1.90                     | 0.52              |
| 1:L:124:VAL:HG21 | 1:L:508:ALA:HB2  | 1.91                     | 0.52              |
| 1:N:13:ARG:HD2   | 1:N:104:LEU:HD22 | 1.91                     | 0.52              |
| 1:B:13:ARG:HD2   | 1:B:104:LEU:HD22 | 1.91                     | 0.52              |
| 1:C:290:GLN:NE2  | 1:C:291:ASP:OD1  | 2.43                     | 0.52              |
| 1:F:13:ARG:HD2   | 1:F:104:LEU:HD22 | 1.91                     | 0.52              |
| 1:F:59:GLU:O     | 1:I:4:LYS:HG3    | 2.10                     | 0.52              |
| 1:J:13:ARG:HD2   | 1:J:104:LEU:HD22 | 1.91                     | 0.52              |
| 1:J:124:VAL:HG21 | 1:J:508:ALA:HB2  | 1.92                     | 0.52              |
| 1:B:320:ALA:HA   | 1:B:335:GLY:HA2  | 1.92                     | 0.52              |
| 1:D:27:VAL:O     | 1:D:30:THR:OG1   | 2.28                     | 0.52              |
| 1:D:362:ARG:NH1  | 1:D:362:ARG:HA   | 2.24                     | 0.52              |
| 1:E:25:ASP:HA    | 1:E:28:LYS:HG2   | 1.92                     | 0.52              |
| 1:J:143:ALA:HB1  | 1:J:146:GLN:HB2  | 1.92                     | 0.52              |
| 1:K:13:ARG:HD2   | 1:K:104:LEU:HD22 | 1.92                     | 0.52              |
| 1:L:353:ILE:O    | 1:L:362:ARG:NH2  | 2.43                     | 0.52              |
| 1:G:185:ASP:HA   | 1:G:380:LYS:O    | 2.10                     | 0.52              |
| 1:G:241:ALA:O    | 1:B:255:GLU:HB2  | 2.09                     | 0.52              |
| 1:H:4:LYS:HG3    | 1:J:59:GLU:O     | 2.10                     | 0.52              |
| 1:J:124:VAL:HG21 | 1:J:508:ALA:CB   | 2.40                     | 0.52              |
| 1:L:200:LEU:HD13 | 1:L:254:VAL:H    | 1.75                     | 0.52              |
| 1:G:218:PRO:HG2  | 1:G:320:ALA:HB3  | 1.92                     | 0.52              |
| 1:B:25:ASP:HA    | 1:B:28:LYS:HG2   | 1.92                     | 0.52              |
| 1:D:320:ALA:HA   | 1:D:335:GLY:HA2  | 1.92                     | 0.52              |
| 1:L:233:MET:HE3  | 1:N:242:LYS:HE2  | 1.91                     | 0.52              |
| 1:J:68:ASN:O     | 1:J:72:GLN:HG2   | 2.10                     | 0.51              |
| 1:K:185:ASP:HA   | 1:K:380:LYS:O    | 2.11                     | 0.51              |
| 1:L:362:ARG:NH1  | 1:L:362:ARG:HA   | 2.25                     | 0.51              |
| 1:N:25:ASP:HA    | 1:N:28:LYS:HG2   | 1.92                     | 0.51              |
| 1:J:106:ALA:O    | 1:J:111:MET:HG3  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:362:ARG:HA   | 1:G:362:ARG:NH1  | 2.25                     | 0.51              |
| 1:A:4:LYS:HG3    | 1:C:59:GLU:O     | 2.10                     | 0.51              |
| 1:K:31:LEU:HD23  | 1:K:453:GLN:HB3  | 1.92                     | 0.51              |
| 1:A:124:VAL:HG21 | 1:A:508:ALA:HB2  | 1.91                     | 0.51              |
| 1:B:219:PHE:N    | 1:B:246:PRO:O    | 2.38                     | 0.51              |
| 1:D:124:VAL:HG21 | 1:D:508:ALA:HB2  | 1.92                     | 0.51              |
| 1:E:168:LYS:HD2  | 1:E:189:VAL:HG21 | 1.92                     | 0.51              |
| 1:B:59:GLU:O     | 1:D:4:LYS:HG3    | 2.11                     | 0.51              |
| 1:E:31:LEU:HD23  | 1:E:453:GLN:HB3  | 1.92                     | 0.51              |
| 1:F:124:VAL:HG21 | 1:F:508:ALA:CB   | 2.41                     | 0.51              |
| 1:H:23:LEU:HD22  | 1:H:74:VAL:HG12  | 1.92                     | 0.51              |
| 1:J:200:LEU:HD21 | 1:J:277:LYS:HG3  | 1.91                     | 0.51              |
| 1:L:13:ARG:NH1   | 1:L:518:GLU:OE1  | 2.38                     | 0.51              |
| 1:L:195:PHE:HB2  | 1:L:279:PRO:HG3  | 1.92                     | 0.51              |
| 1:L:361:ASP:HA   | 1:L:364:LYS:HG2  | 1.91                     | 0.51              |
| 1:B:124:VAL:HG21 | 1:B:508:ALA:HB2  | 1.91                     | 0.51              |
| 1:D:143:ALA:HB1  | 1:D:146:GLN:HB2  | 1.93                     | 0.51              |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:HB2  | 1.91                     | 0.51              |
| 1:H:361:ASP:HA   | 1:H:364:LYS:HE3  | 1.93                     | 0.51              |
| 1:I:106:ALA:O    | 1:I:111:MET:HG3  | 2.11                     | 0.51              |
| 1:K:288:MET:HE1  | 1:K:368:ARG:HG2  | 1.92                     | 0.51              |
| 1:K:361:ASP:HA   | 1:K:364:LYS:HE3  | 1.93                     | 0.51              |
| 1:G:4:LYS:HG3    | 1:M:59:GLU:O     | 2.11                     | 0.51              |
| 1:G:124:VAL:HG21 | 1:G:508:ALA:HB2  | 1.91                     | 0.51              |
| 1:N:124:VAL:HG21 | 1:N:508:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:365:LEU:O    | 1:A:369:VAL:HG22 | 2.11                     | 0.51              |
| 1:I:241:ALA:O    | 1:K:255:GLU:HB2  | 2.10                     | 0.51              |
| 1:L:4:LYS:HG3    | 1:N:59:GLU:O     | 2.11                     | 0.51              |
| 1:A:59:GLU:O     | 1:N:4:LYS:HG3    | 2.11                     | 0.51              |
| 1:B:23:LEU:HD22  | 1:B:74:VAL:HG12  | 1.92                     | 0.51              |
| 1:B:113:PRO:HA   | 1:B:116:LEU:HD12 | 1.93                     | 0.51              |
| 1:C:288:MET:N    | 1:C:288:MET:HE2  | 2.26                     | 0.51              |
| 1:F:150:ILE:HG13 | 1:F:493:ILE:HA   | 1.93                     | 0.51              |
| 1:H:118:ARG:NH2  | 5:H:716:HOH:O    | 2.44                     | 0.51              |
| 1:K:236:VAL:HG21 | 1:K:309:LEU:HB3  | 1.91                     | 0.51              |
| 1:L:421:ARG:NH2  | 1:L:476:TYR:O    | 2.43                     | 0.51              |
| 1:C:143:ALA:HB1  | 1:C:146:GLN:HB2  | 1.92                     | 0.51              |
| 1:F:230:ILE:HD11 | 1:F:258:ALA:HB1  | 1.92                     | 0.51              |
| 1:I:288:MET:HE2  | 1:I:288:MET:N    | 2.26                     | 0.51              |
| 1:N:31:LEU:O     | 1:N:457:ASN:ND2  | 2.41                     | 0.51              |
| 1:N:168:LYS:HD2  | 1:N:189:VAL:HG21 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:361:ASP:HA   | 1:G:364:LYS:HE3  | 1.93                     | 0.50              |
| 1:I:143:ALA:HB1  | 1:I:146:GLN:HB2  | 1.94                     | 0.50              |
| 1:K:118:ARG:NH2  | 5:K:716:HOH:O    | 2.44                     | 0.50              |
| 1:L:150:ILE:HG13 | 1:L:493:ILE:HA   | 1.93                     | 0.50              |
| 1:G:59:GLU:O     | 1:B:4:LYS:HG3    | 2.11                     | 0.50              |
| 1:G:213:VAL:HG22 | 1:G:325:ILE:HB   | 1.93                     | 0.50              |
| 1:C:261:THR:HG21 | 1:E:267:MET:HA   | 1.93                     | 0.50              |
| 1:E:124:VAL:HG21 | 1:E:508:ALA:CB   | 2.40                     | 0.50              |
| 1:K:221:LEU:HD23 | 1:K:249:ILE:HG12 | 1.94                     | 0.50              |
| 1:L:114:MET:HE3  | 1:L:117:LYS:HD3  | 1.93                     | 0.50              |
| 1:L:290:GLN:NE2  | 1:L:291:ASP:OD1  | 2.44                     | 0.50              |
| 1:N:361:ASP:HA   | 1:N:364:LYS:HE3  | 1.93                     | 0.50              |
| 1:F:218:PRO:HG2  | 1:F:320:ALA:HB3  | 1.94                     | 0.50              |
| 1:H:113:PRO:HA   | 1:H:116:LEU:HD12 | 1.92                     | 0.50              |
| 1:H:150:ILE:HG13 | 1:H:493:ILE:HA   | 1.92                     | 0.50              |
| 1:K:40:LEU:HD13  | 1:K:59:GLU:HG3   | 1.93                     | 0.50              |
| 1:K:124:VAL:HG21 | 1:K:508:ALA:CB   | 2.41                     | 0.50              |
| 1:D:150:ILE:HG13 | 1:D:493:ILE:HA   | 1.93                     | 0.50              |
| 1:I:114:MET:HE3  | 1:I:117:LYS:HD3  | 1.92                     | 0.50              |
| 1:A:242:LYS:HE2  | 1:N:226:LYS:HA   | 1.94                     | 0.50              |
| 1:B:31:LEU:O     | 1:B:457:ASN:ND2  | 2.41                     | 0.50              |
| 1:H:320:ALA:HA   | 1:H:335:GLY:HA2  | 1.94                     | 0.50              |
| 1:K:244:GLY:HA3  | 1:M:253:ASP:HB3  | 1.93                     | 0.50              |
| 1:B:68:ASN:O     | 1:B:72:GLN:HG2   | 2.11                     | 0.50              |
| 1:D:487:ASN:O    | 1:D:491:MET:HG3  | 2.12                     | 0.50              |
| 1:F:68:ASN:O     | 1:F:72:GLN:HG2   | 2.12                     | 0.50              |
| 1:H:491:MET:HE3  | 1:H:493:ILE:HD12 | 1.93                     | 0.50              |
| 1:M:362:ARG:CZ   | 1:M:362:ARG:HA   | 2.41                     | 0.50              |
| 1:N:113:PRO:HA   | 1:N:116:LEU:HD12 | 1.94                     | 0.50              |
| 1:N:366:GLN:HA   | 1:N:369:VAL:HG22 | 1.93                     | 0.50              |
| 1:G:255:GLU:HG2  | 1:M:244:GLY:H    | 1.76                     | 0.50              |
| 1:D:361:ASP:HA   | 1:D:364:LYS:HE3  | 1.94                     | 0.50              |
| 1:E:40:LEU:HD13  | 1:E:59:GLU:HG3   | 1.94                     | 0.50              |
| 1:H:349:ILE:O    | 1:H:353:ILE:HG13 | 2.12                     | 0.50              |
| 1:I:150:ILE:HG13 | 1:I:493:ILE:HA   | 1.93                     | 0.50              |
| 1:K:363:GLU:O    | 1:K:366:GLN:HG2  | 2.12                     | 0.50              |
| 1:M:13:ARG:HD2   | 1:M:104:LEU:HD22 | 1.94                     | 0.50              |
| 1:M:143:ALA:HB1  | 1:M:146:GLN:HB2  | 1.92                     | 0.50              |
| 1:N:215:LEU:HB3  | 1:N:218:PRO:HB3  | 1.94                     | 0.50              |
| 1:C:323:VAL:HG22 | 1:C:332:ILE:HA   | 1.94                     | 0.50              |
| 1:E:320:ALA:HA   | 1:E:335:GLY:HA2  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:150:ILE:HG13 | 1:J:493:ILE:HA   | 1.93                     | 0.50              |
| 1:J:278:ALA:HB3  | 1:J:285:ARG:HH11 | 1.76                     | 0.50              |
| 1:F:320:ALA:HA   | 1:F:335:GLY:HA2  | 1.94                     | 0.50              |
| 1:H:56:VAL:O     | 1:H:60:ILE:HG12  | 2.12                     | 0.50              |
| 1:J:288:MET:SD   | 1:J:289:LEU:N    | 2.85                     | 0.50              |
| 1:J:290:GLN:NE2  | 1:J:291:ASP:OD1  | 2.44                     | 0.50              |
| 1:L:68:ASN:O     | 1:L:72:GLN:HG2   | 2.11                     | 0.50              |
| 1:G:225:LYS:HD3  | 1:G:303:GLU:HG3  | 1.93                     | 0.49              |
| 1:A:219:PHE:HD1  | 1:A:245:LYS:HD2  | 1.77                     | 0.49              |
| 1:A:417:VAL:HG21 | 1:A:477:GLY:HA3  | 1.94                     | 0.49              |
| 1:D:244:GLY:HA2  | 1:F:255:GLU:HG2  | 1.94                     | 0.49              |
| 1:E:325:ILE:HA   | 1:E:330:THR:HG23 | 1.94                     | 0.49              |
| 1:G:124:VAL:HG21 | 1:G:508:ALA:CB   | 2.42                     | 0.49              |
| 1:G:191:GLU:HG2  | 1:G:342:ILE:HD13 | 1.93                     | 0.49              |
| 1:G:417:VAL:HG21 | 1:G:477:GLY:HA3  | 1.94                     | 0.49              |
| 1:A:124:VAL:HG21 | 1:A:508:ALA:CB   | 2.42                     | 0.49              |
| 1:H:25:ASP:HA    | 1:H:28:LYS:HG2   | 1.94                     | 0.49              |
| 1:H:302:SER:OG   | 1:H:304:GLU:OE2  | 2.29                     | 0.49              |
| 1:I:206:ASN:HB3  | 1:I:208:PRO:HD2  | 1.94                     | 0.49              |
| 1:I:362:ARG:NH1  | 1:I:362:ARG:HA   | 2.27                     | 0.49              |
| 1:G:200:LEU:HD21 | 1:G:277:LYS:HG3  | 1.94                     | 0.49              |
| 1:G:411:VAL:HG21 | 1:G:494:LEU:HD23 | 1.94                     | 0.49              |
| 1:B:222:LEU:HB3  | 1:B:289:LEU:HD12 | 1.93                     | 0.49              |
| 1:C:68:ASN:O     | 1:C:72:GLN:HG2   | 2.11                     | 0.49              |
| 1:E:68:ASN:O     | 1:E:72:GLN:HG2   | 2.12                     | 0.49              |
| 1:F:221:LEU:HD23 | 1:F:249:ILE:HG12 | 1.93                     | 0.49              |
| 1:I:200:LEU:HD21 | 1:I:277:LYS:HG3  | 1.93                     | 0.49              |
| 1:I:417:VAL:HG21 | 1:I:477:GLY:HA3  | 1.93                     | 0.49              |
| 1:I:487:ASN:O    | 1:I:491:MET:HG3  | 2.12                     | 0.49              |
| 1:J:195:PHE:HB2  | 1:J:279:PRO:HG3  | 1.95                     | 0.49              |
| 1:L:516:THR:OG1  | 1:N:37:ASN:ND2   | 2.39                     | 0.49              |
| 1:G:27:VAL:HG12  | 1:G:90:THR:HG23  | 1.95                     | 0.49              |
| 1:C:13:ARG:HD2   | 1:C:104:LEU:HD22 | 1.94                     | 0.49              |
| 1:D:361:ASP:HA   | 1:D:364:LYS:HG2  | 1.94                     | 0.49              |
| 1:I:56:VAL:O     | 1:I:60:ILE:HG12  | 2.13                     | 0.49              |
| 1:I:491:MET:HE3  | 1:I:493:ILE:HD12 | 1.93                     | 0.49              |
| 1:L:411:VAL:HG21 | 1:L:494:LEU:HD23 | 1.94                     | 0.49              |
| 1:G:13:ARG:HD2   | 1:G:104:LEU:HD22 | 1.94                     | 0.49              |
| 1:G:113:PRO:HA   | 1:G:116:LEU:HD12 | 1.94                     | 0.49              |
| 1:A:68:ASN:O     | 1:A:72:GLN:HG2   | 2.12                     | 0.49              |
| 1:B:361:ASP:HA   | 1:B:364:LYS:HE3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:27:VAL:O     | 1:C:30:THR:OG1   | 2.26                     | 0.49              |
| 1:L:247:LEU:HB3  | 1:L:273:VAL:HG22 | 1.95                     | 0.49              |
| 1:M:185:ASP:HA   | 1:M:380:LYS:O    | 2.12                     | 0.49              |
| 1:N:225:LYS:HD3  | 1:N:303:GLU:HG3  | 1.94                     | 0.49              |
| 1:A:13:ARG:HD2   | 1:A:104:LEU:HD22 | 1.94                     | 0.49              |
| 1:D:218:PRO:HG2  | 1:D:320:ALA:HB3  | 1.95                     | 0.49              |
| 1:D:417:VAL:HG21 | 1:D:477:GLY:HA3  | 1.94                     | 0.49              |
| 1:I:23:LEU:HD22  | 1:I:74:VAL:HG12  | 1.94                     | 0.49              |
| 1:I:37:ASN:ND2   | 1:K:516:THR:OG1  | 2.42                     | 0.49              |
| 1:I:68:ASN:O     | 1:I:72:GLN:HG2   | 2.11                     | 0.49              |
| 1:K:31:LEU:O     | 1:K:457:ASN:ND2  | 2.35                     | 0.49              |
| 1:M:361:ASP:HA   | 1:M:364:LYS:HE3  | 1.93                     | 0.49              |
| 1:A:221:LEU:HD23 | 1:A:249:ILE:HG12 | 1.93                     | 0.49              |
| 1:A:428:ASP:OD1  | 1:A:428:ASP:N    | 2.42                     | 0.49              |
| 1:C:124:VAL:HG21 | 1:C:508:ALA:CB   | 2.43                     | 0.49              |
| 1:C:233:MET:SD   | 1:C:237:LEU:HG   | 2.52                     | 0.49              |
| 1:D:59:GLU:O     | 1:F:4:LYS:HG3    | 2.13                     | 0.49              |
| 1:E:31:LEU:O     | 1:E:457:ASN:ND2  | 2.36                     | 0.49              |
| 1:E:56:VAL:O     | 1:E:60:ILE:HG12  | 2.12                     | 0.49              |
| 1:F:106:ALA:O    | 1:F:111:MET:HG3  | 2.13                     | 0.49              |
| 1:I:382:GLY:O    | 1:I:392:LYS:NZ   | 2.36                     | 0.49              |
| 1:K:56:VAL:O     | 1:K:60:ILE:HG12  | 2.12                     | 0.49              |
| 1:M:68:ASN:O     | 1:M:72:GLN:HG2   | 2.12                     | 0.49              |
| 1:M:218:PRO:HG2  | 1:M:320:ALA:HB3  | 1.95                     | 0.49              |
| 1:A:25:ASP:HA    | 1:A:28:LYS:HG2   | 1.95                     | 0.49              |
| 1:C:225:LYS:HD2  | 1:C:303:GLU:HG3  | 1.94                     | 0.49              |
| 1:E:226:LYS:NZ   | 1:E:253:ASP:O    | 2.35                     | 0.49              |
| 1:E:362:ARG:CZ   | 1:E:362:ARG:HA   | 2.43                     | 0.49              |
| 1:H:68:ASN:O     | 1:H:72:GLN:HG2   | 2.11                     | 0.49              |
| 1:I:25:ASP:HA    | 1:I:28:LYS:HG2   | 1.95                     | 0.49              |
| 1:H:498:LYS:HG3  | 1:H:501:ARG:HH21 | 1.78                     | 0.49              |
| 1:J:366:GLN:HA   | 1:J:369:VAL:HG12 | 1.95                     | 0.49              |
| 1:M:124:VAL:HG21 | 1:M:508:ALA:CB   | 2.43                     | 0.49              |
| 1:D:124:VAL:HG21 | 1:D:508:ALA:CB   | 2.43                     | 0.49              |
| 1:D:362:ARG:HH12 | 1:D:365:LEU:HD12 | 1.77                     | 0.49              |
| 1:H:256:GLY:HA2  | 1:H:260:ALA:HB3  | 1.95                     | 0.49              |
| 1:J:4:LYS:HG3    | 1:L:59:GLU:O     | 2.13                     | 0.49              |
| 1:J:23:LEU:HD22  | 1:J:74:VAL:HG12  | 1.95                     | 0.49              |
| 1:M:118:ARG:NH2  | 5:M:720:HOH:O    | 2.45                     | 0.49              |
| 1:M:362:ARG:HA   | 1:M:362:ARG:NE   | 2.28                     | 0.49              |
| 1:G:68:ASN:O     | 1:G:72:GLN:HG2   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:151:SER:HB3  | 1:G:399:ALA:HA   | 1.95                     | 0.48              |
| 1:D:25:ASP:HA    | 1:D:28:LYS:HG2   | 1.95                     | 0.48              |
| 1:D:207:LYS:NZ   | 5:D:704:HOH:O    | 2.31                     | 0.48              |
| 1:J:417:VAL:HG21 | 1:J:477:GLY:HA3  | 1.94                     | 0.48              |
| 1:K:68:ASN:O     | 1:K:72:GLN:HG2   | 2.11                     | 0.48              |
| 1:L:487:ASN:O    | 1:L:491:MET:HG3  | 2.13                     | 0.48              |
| 1:G:25:ASP:HA    | 1:G:28:LYS:HG2   | 1.96                     | 0.48              |
| 1:G:144:ILE:HG21 | 1:G:166:MET:HE2  | 1.95                     | 0.48              |
| 1:A:193:MET:HB2  | 1:A:295:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:428:ASP:OD1  | 1:B:428:ASP:N    | 2.43                     | 0.48              |
| 1:C:151:SER:HB3  | 1:C:399:ALA:HA   | 1.96                     | 0.48              |
| 1:D:193:MET:HE1  | 1:D:371:LYS:HB3  | 1.95                     | 0.48              |
| 1:F:361:ASP:HA   | 1:F:364:LYS:HG2  | 1.95                     | 0.48              |
| 1:H:417:VAL:HG21 | 1:H:477:GLY:HA3  | 1.93                     | 0.48              |
| 1:I:113:PRO:HA   | 1:I:116:LEU:HD12 | 1.94                     | 0.48              |
| 1:M:200:LEU:HD21 | 1:M:277:LYS:HG3  | 1.95                     | 0.48              |
| 1:G:428:ASP:OD1  | 1:G:428:ASP:N    | 2.42                     | 0.48              |
| 1:A:226:LYS:HE3  | 1:C:242:LYS:HE3  | 1.95                     | 0.48              |
| 1:A:513:LEU:HD23 | 1:A:513:LEU:HA   | 1.72                     | 0.48              |
| 1:D:218:PRO:HG3  | 1:D:323:VAL:HB   | 1.95                     | 0.48              |
| 1:I:142:LYS:NZ   | 5:I:706:HOH:O    | 2.42                     | 0.48              |
| 1:I:244:GLY:HA3  | 1:K:253:ASP:HB3  | 1.95                     | 0.48              |
| 1:K:417:VAL:HG21 | 1:K:477:GLY:HA3  | 1.95                     | 0.48              |
| 1:F:362:ARG:HA   | 1:F:362:ARG:NH1  | 2.29                     | 0.48              |
| 1:I:31:LEU:HD23  | 1:I:453:GLN:HB3  | 1.96                     | 0.48              |
| 1:I:124:VAL:HG21 | 1:I:508:ALA:CB   | 2.43                     | 0.48              |
| 1:J:144:ILE:HG21 | 1:J:166:MET:SD   | 2.52                     | 0.48              |
| 1:J:176:THR:HG21 | 1:J:333:ILE:HD11 | 1.94                     | 0.48              |
| 1:L:25:ASP:HA    | 1:L:28:LYS:HG2   | 1.95                     | 0.48              |
| 1:C:150:ILE:HG13 | 1:C:493:ILE:HA   | 1.94                     | 0.48              |
| 1:D:68:ASN:O     | 1:D:72:GLN:HG2   | 2.13                     | 0.48              |
| 1:H:124:VAL:HG21 | 1:H:508:ALA:CB   | 2.43                     | 0.48              |
| 1:L:124:VAL:HG21 | 1:L:508:ALA:CB   | 2.43                     | 0.48              |
| 1:M:27:VAL:O     | 1:M:30:THR:OG1   | 2.26                     | 0.48              |
| 1:G:244:GLY:HA3  | 1:B:253:ASP:HB3  | 1.96                     | 0.48              |
| 1:G:271:VAL:HG21 | 1:B:255:GLU:HB3  | 1.94                     | 0.48              |
| 1:G:361:ASP:HA   | 1:G:364:LYS:HG2  | 1.95                     | 0.48              |
| 1:G:516:THR:OG1  | 1:M:37:ASN:ND2   | 2.43                     | 0.48              |
| 1:A:151:SER:HB3  | 1:A:399:ALA:HA   | 1.96                     | 0.48              |
| 1:C:168:LYS:HD2  | 1:C:189:VAL:HG21 | 1.95                     | 0.48              |
| 1:F:185:ASP:HA   | 1:F:380:LYS:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:27:VAL:O     | 1:H:30:THR:OG1   | 2.26                     | 0.48              |
| 1:I:219:PHE:N    | 1:I:246:PRO:O    | 2.36                     | 0.48              |
| 1:L:69:MET:HE3   | 1:L:520:MET:HE2  | 1.95                     | 0.48              |
| 1:B:268:ARG:HH11 | 1:D:264:VAL:HG11 | 1.79                     | 0.48              |
| 1:H:365:LEU:HD23 | 1:H:368:ARG:HD3  | 1.95                     | 0.48              |
| 1:J:361:ASP:HA   | 1:J:364:LYS:HG2  | 1.96                     | 0.48              |
| 1:L:417:VAL:HG21 | 1:L:477:GLY:HA3  | 1.94                     | 0.48              |
| 1:N:382:GLY:O    | 1:N:392:LYS:NZ   | 2.36                     | 0.48              |
| 1:G:175:ILE:HG12 | 1:G:377:ALA:HB3  | 1.95                     | 0.48              |
| 1:B:213:VAL:HG22 | 1:B:325:ILE:HB   | 1.95                     | 0.48              |
| 1:C:411:VAL:HG21 | 1:C:494:LEU:HD23 | 1.96                     | 0.48              |
| 1:H:31:LEU:HD23  | 1:H:453:GLN:HB3  | 1.96                     | 0.48              |
| 1:L:456:LEU:HG   | 1:L:462:PRO:HG3  | 1.96                     | 0.48              |
| 1:G:150:ILE:HG13 | 1:G:493:ILE:HA   | 1.95                     | 0.48              |
| 1:A:240:VAL:HG11 | 1:A:247:LEU:HB2  | 1.96                     | 0.48              |
| 1:F:197:ARG:HH21 | 1:F:279:PRO:HA   | 1.79                     | 0.48              |
| 1:H:180:GLY:HA2  | 1:H:380:LYS:HD2  | 1.95                     | 0.48              |
| 1:I:361:ASP:HA   | 1:I:364:LYS:HG2  | 1.96                     | 0.48              |
| 1:K:353:ILE:HG13 | 1:K:365:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:111:MET:SD   | 1:B:438:VAL:HG11 | 2.54                     | 0.48              |
| 1:B:244:GLY:HA2  | 1:D:255:GLU:HG3  | 1.96                     | 0.48              |
| 1:D:31:LEU:O     | 1:D:457:ASN:ND2  | 2.41                     | 0.48              |
| 1:E:150:ILE:HG13 | 1:E:493:ILE:HA   | 1.96                     | 0.48              |
| 1:E:353:ILE:HG21 | 1:E:366:GLN:HE22 | 1.79                     | 0.48              |
| 1:K:113:PRO:HA   | 1:K:116:LEU:HD12 | 1.95                     | 0.48              |
| 1:G:487:ASN:O    | 1:G:491:MET:HG3  | 2.14                     | 0.47              |
| 1:A:150:ILE:HG13 | 1:A:493:ILE:HA   | 1.95                     | 0.47              |
| 1:A:255:GLU:HB2  | 1:C:241:ALA:O    | 2.14                     | 0.47              |
| 1:C:118:ARG:NH2  | 5:C:717:HOH:O    | 2.47                     | 0.47              |
| 1:F:25:ASP:HA    | 1:F:28:LYS:HG2   | 1.96                     | 0.47              |
| 1:H:487:ASN:O    | 1:H:491:MET:HG3  | 2.14                     | 0.47              |
| 1:I:151:SER:HB3  | 1:I:399:ALA:HA   | 1.95                     | 0.47              |
| 1:L:168:LYS:HD2  | 1:L:189:VAL:HG21 | 1.96                     | 0.47              |
| 1:M:180:GLY:HA2  | 1:M:380:LYS:HD2  | 1.96                     | 0.47              |
| 1:A:288:MET:HE1  | 1:A:368:ARG:HD2  | 1.96                     | 0.47              |
| 1:D:74:VAL:CG1   | 1:D:514:MET:HE1  | 2.43                     | 0.47              |
| 1:E:417:VAL:HG21 | 1:E:477:GLY:HA3  | 1.96                     | 0.47              |
| 1:F:356:ALA:O    | 1:F:362:ARG:NH2  | 2.48                     | 0.47              |
| 1:H:13:ARG:HD2   | 1:H:104:LEU:HD22 | 1.96                     | 0.47              |
| 1:N:213:VAL:HG22 | 1:N:325:ILE:HB   | 1.96                     | 0.47              |
| 1:A:487:ASN:O    | 1:A:491:MET:HG3  | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:ILE:HD12 | 1:B:275:ALA:HB2  | 1.96                     | 0.47              |
| 1:I:13:ARG:NH1   | 1:I:518:GLU:OE1  | 2.35                     | 0.47              |
| 1:J:135:SER:O    | 5:J:701:HOH:O    | 2.20                     | 0.47              |
| 1:K:428:ASP:OD1  | 1:K:428:ASP:N    | 2.36                     | 0.47              |
| 1:N:180:GLY:HA2  | 1:N:380:LYS:HD2  | 1.96                     | 0.47              |
| 1:H:31:LEU:O     | 1:H:457:ASN:ND2  | 2.36                     | 0.47              |
| 1:A:204:PHE:O    | 1:A:213:VAL:HG11 | 2.14                     | 0.47              |
| 1:C:361:ASP:HA   | 1:C:364:LYS:HG2  | 1.95                     | 0.47              |
| 1:C:362:ARG:NH1  | 1:C:362:ARG:HA   | 2.30                     | 0.47              |
| 1:F:27:VAL:O     | 1:F:30:THR:OG1   | 2.32                     | 0.47              |
| 1:I:31:LEU:O     | 1:I:457:ASN:ND2  | 2.36                     | 0.47              |
| 1:I:287:ALA:HB3  | 1:I:288:MET:HE2  | 1.96                     | 0.47              |
| 1:L:321:LYS:HB3  | 1:L:334:ASP:HB3  | 1.96                     | 0.47              |
| 1:N:428:ASP:OD1  | 1:N:428:ASP:N    | 2.44                     | 0.47              |
| 1:D:114:MET:HE3  | 1:D:117:LYS:HD3  | 1.94                     | 0.47              |
| 1:E:177:VAL:HG23 | 1:E:400:LEU:HD22 | 1.96                     | 0.47              |
| 1:E:322:ARG:HB3  | 1:E:333:ILE:HB   | 1.96                     | 0.47              |
| 1:I:239:ALA:HB1  | 1:I:314:LEU:HD21 | 1.97                     | 0.47              |
| 1:J:25:ASP:HA    | 1:J:28:LYS:HG2   | 1.97                     | 0.47              |
| 1:N:411:VAL:HG21 | 1:N:494:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:143:ALA:HB1  | 1:G:146:GLN:HB2  | 1.96                     | 0.47              |
| 1:G:253:ASP:HB3  | 1:M:244:GLY:HA3  | 1.96                     | 0.47              |
| 1:A:31:LEU:O     | 1:A:457:ASN:ND2  | 2.36                     | 0.47              |
| 1:A:142:LYS:HD2  | 1:A:142:LYS:HA   | 1.75                     | 0.47              |
| 1:B:124:VAL:HG21 | 1:B:508:ALA:CB   | 2.44                     | 0.47              |
| 1:B:151:SER:HB3  | 1:B:399:ALA:HA   | 1.96                     | 0.47              |
| 1:C:417:VAL:HG21 | 1:C:477:GLY:HA3  | 1.97                     | 0.47              |
| 1:D:411:VAL:HG21 | 1:D:494:LEU:HD23 | 1.97                     | 0.47              |
| 1:F:288:MET:SD   | 1:F:289:LEU:HG   | 2.55                     | 0.47              |
| 1:H:151:SER:HB3  | 1:H:399:ALA:HA   | 1.96                     | 0.47              |
| 1:H:304:GLU:OE2  | 1:H:304:GLU:N    | 2.27                     | 0.47              |
| 1:H:411:VAL:HG21 | 1:H:494:LEU:HD23 | 1.97                     | 0.47              |
| 1:I:13:ARG:HD2   | 1:I:104:LEU:HD22 | 1.96                     | 0.47              |
| 1:I:27:VAL:O     | 1:I:30:THR:OG1   | 2.26                     | 0.47              |
| 1:J:151:SER:HB3  | 1:J:399:ALA:HA   | 1.96                     | 0.47              |
| 1:L:31:LEU:O     | 1:L:457:ASN:ND2  | 2.41                     | 0.47              |
| 1:M:221:LEU:HD23 | 1:M:249:ILE:HG12 | 1.96                     | 0.47              |
| 1:N:124:VAL:HG21 | 1:N:508:ALA:CB   | 2.44                     | 0.47              |
| 1:N:365:LEU:O    | 1:N:369:VAL:HG13 | 2.14                     | 0.47              |
| 1:G:40:LEU:HD13  | 1:G:59:GLU:HG3   | 1.97                     | 0.47              |
| 1:A:362:ARG:CZ   | 1:A:362:ARG:HA   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:ALA:O    | 1:B:111:MET:HG3  | 2.14                     | 0.47              |
| 1:C:287:ALA:HB3  | 1:C:288:MET:HE2  | 1.96                     | 0.47              |
| 1:E:113:PRO:HA   | 1:E:116:LEU:HD12 | 1.96                     | 0.47              |
| 1:K:365:LEU:O    | 1:K:369:VAL:HG22 | 2.15                     | 0.47              |
| 1:M:417:VAL:HG21 | 1:M:477:GLY:HA3  | 1.97                     | 0.47              |
| 1:N:349:ILE:O    | 1:N:353:ILE:HG23 | 2.14                     | 0.47              |
| 1:F:102:GLU:HB3  | 1:F:442:VAL:HG22 | 1.97                     | 0.47              |
| 1:F:118:ARG:NH2  | 5:F:716:HOH:O    | 2.46                     | 0.47              |
| 1:I:180:GLY:HA2  | 1:I:380:LYS:HD2  | 1.96                     | 0.47              |
| 1:E:207:LYS:NZ   | 5:E:713:HOH:O    | 2.41                     | 0.47              |
| 1:I:498:LYS:HG3  | 1:I:501:ARG:HH21 | 1.80                     | 0.47              |
| 1:J:27:VAL:O     | 1:J:30:THR:OG1   | 2.33                     | 0.47              |
| 1:B:479:ASN:HB2  | 1:B:491:MET:CE   | 2.45                     | 0.46              |
| 1:C:100:ILE:HD11 | 1:C:514:MET:HB2  | 1.96                     | 0.46              |
| 1:F:417:VAL:HG21 | 1:F:477:GLY:HA3  | 1.95                     | 0.46              |
| 1:H:13:ARG:NH1   | 1:H:518:GLU:OE1  | 2.36                     | 0.46              |
| 1:K:385:THR:HG21 | 1:M:510:VAL:HG23 | 1.97                     | 0.46              |
| 1:G:240:VAL:HG11 | 1:G:247:LEU:HD22 | 1.96                     | 0.46              |
| 1:B:180:GLY:HA2  | 1:B:380:LYS:HD2  | 1.97                     | 0.46              |
| 1:D:70:GLY:O     | 1:D:74:VAL:HG22  | 2.15                     | 0.46              |
| 1:E:231:ARG:HD3  | 1:E:234:LEU:HD12 | 1.97                     | 0.46              |
| 1:F:361:ASP:HA   | 1:F:364:LYS:HE3  | 1.97                     | 0.46              |
| 1:I:218:PRO:HG2  | 1:I:320:ALA:HB3  | 1.97                     | 0.46              |
| 1:A:244:GLY:N    | 1:N:253:ASP:HB3  | 2.30                     | 0.46              |
| 1:B:142:LYS:HD2  | 1:B:142:LYS:HA   | 1.67                     | 0.46              |
| 1:C:321:LYS:N    | 1:C:334:ASP:O    | 2.36                     | 0.46              |
| 1:D:100:ILE:HD11 | 1:D:514:MET:HE3  | 1.97                     | 0.46              |
| 1:E:118:ARG:NH2  | 5:E:720:HOH:O    | 2.48                     | 0.46              |
| 1:M:411:VAL:HG21 | 1:M:494:LEU:HD23 | 1.98                     | 0.46              |
| 1:A:206:ASN:H    | 1:A:213:VAL:HG12 | 1.80                     | 0.46              |
| 1:A:411:VAL:HG21 | 1:A:494:LEU:HD23 | 1.98                     | 0.46              |
| 1:B:150:ILE:HG13 | 1:B:493:ILE:HA   | 1.97                     | 0.46              |
| 1:F:200:LEU:HD21 | 1:F:277:LYS:HG3  | 1.97                     | 0.46              |
| 1:I:59:GLU:O     | 1:K:4:LYS:HG3    | 2.16                     | 0.46              |
| 1:B:288:MET:HE1  | 1:B:368:ARG:HG2  | 1.98                     | 0.46              |
| 1:H:421:ARG:NH2  | 1:H:476:TYR:O    | 2.48                     | 0.46              |
| 1:N:176:THR:HG21 | 1:N:333:ILE:HD11 | 1.98                     | 0.46              |
| 1:G:279:PRO:HG2  | 1:G:288:MET:HG3  | 1.97                     | 0.46              |
| 1:E:288:MET:SD   | 1:E:288:MET:N    | 2.89                     | 0.46              |
| 1:I:325:ILE:HA   | 1:I:330:THR:HG23 | 1.96                     | 0.46              |
| 1:L:349:ILE:HG23 | 1:L:365:LEU:HD22 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:257:GLU:HB2  | 1:M:267:MET:HG2  | 1.96                     | 0.46              |
| 1:F:411:VAL:HG21 | 1:F:494:LEU:HD23 | 1.97                     | 0.46              |
| 1:H:236:VAL:HG21 | 1:H:309:LEU:HB3  | 1.97                     | 0.46              |
| 1:I:142:LYS:HA   | 1:I:142:LYS:HD2  | 1.64                     | 0.46              |
| 1:M:321:LYS:HB3  | 1:M:334:ASP:HB3  | 1.98                     | 0.46              |
| 1:M:356:ALA:HB3  | 1:M:362:ARG:HH12 | 1.79                     | 0.46              |
| 1:B:417:VAL:HG21 | 1:B:477:GLY:HA3  | 1.97                     | 0.46              |
| 1:C:126:ALA:O    | 1:C:130:GLU:HG2  | 2.16                     | 0.46              |
| 1:D:40:LEU:HD13  | 1:D:59:GLU:HG3   | 1.97                     | 0.46              |
| 1:K:150:ILE:HG13 | 1:K:493:ILE:HA   | 1.98                     | 0.46              |
| 1:K:151:SER:HB3  | 1:K:399:ALA:HA   | 1.98                     | 0.46              |
| 1:L:16:MET:SD    | 1:L:514:MET:HE3  | 2.56                     | 0.46              |
| 1:M:19:GLY:HA3   | 1:M:67:GLU:O     | 2.16                     | 0.46              |
| 1:M:23:LEU:HD22  | 1:M:74:VAL:HG12  | 1.96                     | 0.46              |
| 1:A:31:LEU:HD23  | 1:A:453:GLN:HB3  | 1.98                     | 0.46              |
| 1:A:242:LYS:HG3  | 1:N:226:LYS:HE3  | 1.97                     | 0.46              |
| 1:C:321:LYS:HB3  | 1:C:334:ASP:HB3  | 1.98                     | 0.46              |
| 1:J:456:LEU:HG   | 1:J:462:PRO:HG3  | 1.98                     | 0.46              |
| 1:K:361:ASP:HA   | 1:K:364:LYS:HG2  | 1.98                     | 0.46              |
| 1:G:193:MET:HE1  | 1:G:195:PHE:HB3  | 1.97                     | 0.46              |
| 1:E:4:LYS:HG3    | 1:H:59:GLU:O     | 2.16                     | 0.46              |
| 1:K:268:ARG:HH11 | 1:M:264:VAL:HG11 | 1.81                     | 0.46              |
| 1:M:226:LYS:HA   | 1:M:226:LYS:HD3  | 1.66                     | 0.46              |
| 1:M:456:LEU:HG   | 1:M:462:PRO:HG3  | 1.97                     | 0.46              |
| 1:B:179:ASP:N    | 1:B:179:ASP:OD1  | 2.49                     | 0.45              |
| 1:D:452:ARG:NH2  | 1:D:463:SER:OG   | 2.50                     | 0.45              |
| 1:F:244:GLY:HA3  | 1:I:253:ASP:HB3  | 1.98                     | 0.45              |
| 1:F:353:ILE:HG12 | 1:F:365:LEU:HB3  | 1.98                     | 0.45              |
| 1:I:411:VAL:HG21 | 1:I:494:LEU:HD23 | 1.97                     | 0.45              |
| 1:J:102:GLU:HB3  | 1:J:442:VAL:HG22 | 1.98                     | 0.45              |
| 1:M:242:LYS:HA   | 1:M:242:LYS:HD3  | 1.69                     | 0.45              |
| 1:G:219:PHE:N    | 1:G:246:PRO:O    | 2.42                     | 0.45              |
| 1:C:19:GLY:HA3   | 1:C:67:GLU:O     | 2.16                     | 0.45              |
| 1:C:456:LEU:HG   | 1:C:462:PRO:HG3  | 1.98                     | 0.45              |
| 1:D:31:LEU:HD23  | 1:D:453:GLN:HB3  | 1.98                     | 0.45              |
| 1:D:288:MET:HE2  | 1:D:288:MET:N    | 2.31                     | 0.45              |
| 1:J:166:MET:HB2  | 1:J:171:LYS:HA   | 1.99                     | 0.45              |
| 1:L:361:ASP:HA   | 1:L:364:LYS:HE3  | 1.98                     | 0.45              |
| 1:N:206:ASN:H    | 1:N:213:VAL:HG12 | 1.82                     | 0.45              |
| 1:B:16:MET:HE2   | 1:B:16:MET:HB3   | 1.87                     | 0.45              |
| 1:B:513:LEU:HA   | 1:B:513:LEU:HD23 | 1.73                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:13:ARG:NH1   | 1:C:518:GLU:OE1  | 2.35                     | 0.45              |
| 1:C:178:GLU:OE2  | 1:C:322:ARG:HG2  | 2.16                     | 0.45              |
| 1:C:278:ALA:HB3  | 1:C:285:ARG:HH11 | 1.81                     | 0.45              |
| 1:E:27:VAL:O     | 1:E:30:THR:OG1   | 2.27                     | 0.45              |
| 1:F:353:ILE:HG13 | 1:F:365:LEU:HD12 | 1.98                     | 0.45              |
| 1:J:13:ARG:NH1   | 1:J:518:GLU:OE1  | 2.35                     | 0.45              |
| 1:J:510:VAL:HG23 | 1:L:385:THR:HG21 | 1.99                     | 0.45              |
| 1:L:288:MET:HE2  | 1:L:288:MET:N    | 2.31                     | 0.45              |
| 1:M:150:ILE:HG13 | 1:M:493:ILE:HA   | 1.98                     | 0.45              |
| 1:N:151:SER:HB3  | 1:N:399:ALA:HA   | 1.98                     | 0.45              |
| 1:N:177:VAL:HG23 | 1:N:400:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:307:MET:HE1  | 1:A:312:ALA:HB2  | 1.97                     | 0.45              |
| 1:I:193:MET:HE1  | 1:I:195:PHE:HB3  | 1.99                     | 0.45              |
| 1:J:31:LEU:O     | 1:J:457:ASN:ND2  | 2.37                     | 0.45              |
| 1:J:419:LEU:HA   | 1:J:422:VAL:HG22 | 1.99                     | 0.45              |
| 1:L:31:LEU:HD23  | 1:L:453:GLN:HB3  | 1.98                     | 0.45              |
| 1:M:175:ILE:HG12 | 1:M:377:ALA:HB3  | 1.99                     | 0.45              |
| 1:N:204:PHE:O    | 1:N:213:VAL:HG11 | 2.17                     | 0.45              |
| 1:D:206:ASN:HD21 | 1:D:272:LYS:HD3  | 1.82                     | 0.45              |
| 1:D:385:THR:HG21 | 1:F:510:VAL:HG23 | 1.99                     | 0.45              |
| 1:E:204:PHE:O    | 1:E:213:VAL:HG11 | 2.17                     | 0.45              |
| 1:F:151:SER:HB3  | 1:F:399:ALA:HA   | 1.98                     | 0.45              |
| 1:F:456:LEU:HG   | 1:F:462:PRO:HG3  | 1.99                     | 0.45              |
| 1:C:353:ILE:O    | 1:C:362:ARG:NH2  | 2.49                     | 0.45              |
| 1:C:382:GLY:O    | 1:C:392:LYS:NZ   | 2.35                     | 0.45              |
| 1:D:19:GLY:HA3   | 1:D:67:GLU:O     | 2.17                     | 0.45              |
| 1:J:320:ALA:HA   | 1:J:335:GLY:HA2  | 1.98                     | 0.45              |
| 1:K:27:VAL:O     | 1:K:30:THR:OG1   | 2.28                     | 0.45              |
| 1:K:325:ILE:HA   | 1:K:330:THR:HG23 | 1.99                     | 0.45              |
| 1:N:417:VAL:HG21 | 1:N:477:GLY:HA3  | 1.98                     | 0.45              |
| 1:D:456:LEU:HG   | 1:D:462:PRO:HG3  | 1.99                     | 0.45              |
| 1:F:419:LEU:HA   | 1:F:422:VAL:HG22 | 1.99                     | 0.45              |
| 1:I:421:ARG:NH2  | 1:I:476:TYR:O    | 2.50                     | 0.45              |
| 1:K:293:ALA:O    | 1:K:298:GLY:N    | 2.50                     | 0.45              |
| 1:M:513:LEU:HD12 | 1:M:513:LEU:HA   | 1.70                     | 0.45              |
| 1:N:27:VAL:O     | 1:N:30:THR:OG1   | 2.26                     | 0.45              |
| 1:N:498:LYS:HG3  | 1:N:501:ARG:HH21 | 1.81                     | 0.45              |
| 1:B:325:ILE:HA   | 1:B:330:THR:HG23 | 1.98                     | 0.45              |
| 1:D:44:PHE:CD1   | 1:D:44:PHE:C     | 2.94                     | 0.45              |
| 1:D:382:GLY:O    | 1:D:392:LYS:NZ   | 2.37                     | 0.45              |
| 1:I:16:MET:HE2   | 1:I:16:MET:HB3   | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:54:VAL:HB    | 1:I:89:THR:HG21  | 1.98                     | 0.45              |
| 1:K:142:LYS:HA   | 1:K:142:LYS:HD2  | 1.73                     | 0.45              |
| 1:K:353:ILE:HG12 | 1:K:362:ARG:NH1  | 2.32                     | 0.45              |
| 1:L:428:ASP:OD1  | 1:L:428:ASP:N    | 2.45                     | 0.45              |
| 1:N:212:ALA:O    | 5:N:701:HOH:O    | 2.20                     | 0.45              |
| 1:N:513:LEU:HA   | 1:N:513:LEU:HD23 | 1.72                     | 0.45              |
| 1:A:255:GLU:HG2  | 1:C:244:GLY:CA   | 2.47                     | 0.45              |
| 1:C:365:LEU:HD23 | 1:C:365:LEU:HA   | 1.86                     | 0.45              |
| 1:H:361:ASP:HA   | 1:H:364:LYS:HG2  | 1.99                     | 0.45              |
| 1:K:244:GLY:HA2  | 1:M:255:GLU:HG2  | 1.99                     | 0.45              |
| 1:N:278:ALA:HB3  | 1:N:285:ARG:HH11 | 1.81                     | 0.45              |
| 1:G:228:SER:O    | 1:M:238:GLU:HB3  | 2.16                     | 0.45              |
| 1:F:113:PRO:HA   | 1:F:116:LEU:HD12 | 1.99                     | 0.45              |
| 1:F:207:LYS:HD2  | 1:F:207:LYS:HA   | 1.74                     | 0.45              |
| 1:H:171:LYS:HB3  | 1:H:171:LYS:HE2  | 1.79                     | 0.45              |
| 1:J:353:ILE:HG13 | 1:J:365:LEU:HD12 | 1.98                     | 0.45              |
| 1:K:216:GLU:HG3  | 1:K:322:ARG:HD2  | 1.98                     | 0.45              |
| 1:K:411:VAL:HG21 | 1:K:494:LEU:HD23 | 1.99                     | 0.45              |
| 1:M:13:ARG:NH1   | 1:M:518:GLU:OE1  | 2.36                     | 0.45              |
| 1:M:201:SER:HB3  | 1:M:204:PHE:CD2  | 2.52                     | 0.45              |
| 1:G:447:MET:HE2  | 1:G:504:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:487:ASN:O    | 1:B:491:MET:HG3  | 2.18                     | 0.44              |
| 1:C:111:MET:SD   | 1:C:438:VAL:HG11 | 2.57                     | 0.44              |
| 1:C:142:LYS:HA   | 1:C:142:LYS:HD2  | 1.71                     | 0.44              |
| 1:E:253:ASP:HB3  | 1:H:244:GLY:HA3  | 1.98                     | 0.44              |
| 1:E:411:VAL:HG21 | 1:E:494:LEU:HD23 | 1.99                     | 0.44              |
| 1:L:113:PRO:HA   | 1:L:116:LEU:HD12 | 1.99                     | 0.44              |
| 1:N:150:ILE:HG13 | 1:N:493:ILE:HA   | 1.99                     | 0.44              |
| 1:N:307:MET:HE1  | 1:N:312:ALA:HB2  | 1.99                     | 0.44              |
| 1:B:69:MET:SD    | 1:B:522:THR:HB   | 2.57                     | 0.44              |
| 1:C:73:MET:HB3   | 1:C:514:MET:SD   | 2.57                     | 0.44              |
| 1:D:248:LEU:HD22 | 1:D:323:VAL:HG11 | 1.99                     | 0.44              |
| 1:F:514:MET:HE2  | 1:F:514:MET:HB3  | 1.91                     | 0.44              |
| 1:I:419:LEU:HA   | 1:I:422:VAL:HG22 | 2.00                     | 0.44              |
| 1:J:118:ARG:NH2  | 5:J:720:HOH:O    | 2.48                     | 0.44              |
| 1:K:229:ASN:OD1  | 1:K:231:ARG:N    | 2.49                     | 0.44              |
| 1:M:69:MET:SD    | 1:M:522:THR:HB   | 2.58                     | 0.44              |
| 1:M:364:LYS:O    | 1:M:368:ARG:HG3  | 2.17                     | 0.44              |
| 1:C:128:VAL:O    | 1:C:132:LYS:HG2  | 2.17                     | 0.44              |
| 1:D:102:GLU:HB3  | 1:D:442:VAL:HG22 | 1.98                     | 0.44              |
| 1:E:201:SER:HB3  | 1:E:204:PHE:CD2  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:321:LYS:N    | 1:E:334:ASP:O    | 2.43                     | 0.44              |
| 1:F:238:GLU:HB3  | 1:I:228:SER:O    | 2.17                     | 0.44              |
| 1:F:478:TYR:OH   | 1:F:483:GLU:OE1  | 2.20                     | 0.44              |
| 1:H:126:ALA:O    | 1:H:130:GLU:HG2  | 2.16                     | 0.44              |
| 1:H:201:SER:HB3  | 1:H:204:PHE:CD2  | 2.53                     | 0.44              |
| 1:I:456:LEU:HG   | 1:I:462:PRO:HG3  | 1.99                     | 0.44              |
| 1:K:102:GLU:HB3  | 1:K:442:VAL:HG22 | 1.98                     | 0.44              |
| 1:M:358:SER:O    | 1:M:362:ARG:N    | 2.44                     | 0.44              |
| 1:B:288:MET:HE3  | 1:B:288:MET:HA   | 1.99                     | 0.44              |
| 1:E:195:PHE:HD2  | 1:E:197:ARG:HB2  | 1.80                     | 0.44              |
| 1:I:513:LEU:HD23 | 1:I:513:LEU:HA   | 1.76                     | 0.44              |
| 1:J:195:PHE:CD2  | 1:J:197:ARG:HB2  | 2.52                     | 0.44              |
| 1:J:478:TYR:OH   | 1:J:483:GLU:OE1  | 2.21                     | 0.44              |
| 1:K:456:LEU:HG   | 1:K:462:PRO:HG3  | 1.99                     | 0.44              |
| 1:N:219:PHE:N    | 1:N:246:PRO:O    | 2.36                     | 0.44              |
| 1:G:207:LYS:HA   | 1:G:207:LYS:HD2  | 1.84                     | 0.44              |
| 1:A:516:THR:OG1  | 1:C:37:ASN:ND2   | 2.40                     | 0.44              |
| 1:C:464:VAL:HG23 | 1:D:463:SER:HB3  | 1.98                     | 0.44              |
| 1:F:218:PRO:HA   | 1:F:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:H:111:MET:SD   | 1:H:438:VAL:HG11 | 2.58                     | 0.44              |
| 1:H:204:PHE:O    | 1:H:272:LYS:HE3  | 2.17                     | 0.44              |
| 1:H:456:LEU:HG   | 1:H:462:PRO:HG3  | 1.99                     | 0.44              |
| 1:J:221:LEU:HD23 | 1:J:249:ILE:HG12 | 2.00                     | 0.44              |
| 1:J:514:MET:HE2  | 1:J:514:MET:HB3  | 1.91                     | 0.44              |
| 1:K:207:LYS:HA   | 1:K:207:LYS:HD2  | 1.75                     | 0.44              |
| 1:K:447:MET:HE2  | 1:K:504:LEU:HD21 | 2.00                     | 0.44              |
| 1:L:19:GLY:HA3   | 1:L:67:GLU:O     | 2.18                     | 0.44              |
| 1:M:293:ALA:O    | 1:M:298:GLY:N    | 2.48                     | 0.44              |
| 1:M:498:LYS:HG3  | 1:M:501:ARG:HH21 | 1.83                     | 0.44              |
| 1:N:111:MET:HE2  | 1:N:111:MET:HB3  | 1.90                     | 0.44              |
| 1:G:28:LYS:HD3   | 1:G:453:GLN:CD   | 2.43                     | 0.44              |
| 1:A:16:MET:HE2   | 1:A:16:MET:HB3   | 1.87                     | 0.44              |
| 1:B:37:ASN:ND2   | 1:D:516:THR:OG1  | 2.43                     | 0.44              |
| 1:C:419:LEU:HA   | 1:C:422:VAL:HG22 | 1.99                     | 0.44              |
| 1:H:54:VAL:HB    | 1:H:89:THR:HG21  | 1.98                     | 0.44              |
| 1:H:160:LYS:HB3  | 1:H:160:LYS:HE3  | 1.68                     | 0.44              |
| 1:J:113:PRO:HA   | 1:J:116:LEU:HD12 | 2.00                     | 0.44              |
| 1:J:195:PHE:HD2  | 1:J:197:ARG:HB2  | 1.83                     | 0.44              |
| 1:L:422:VAL:HG23 | 1:L:447:MET:HE3  | 1.99                     | 0.44              |
| 1:A:113:PRO:HA   | 1:A:116:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:447:MET:HE2  | 1:A:504:LEU:HD21 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:ASN:OD1  | 1:B:230:ILE:N    | 2.51                     | 0.44              |
| 1:C:174:VAL:HG13 | 1:C:376:VAL:HA   | 2.00                     | 0.44              |
| 1:C:510:VAL:HG23 | 1:E:385:THR:HG21 | 2.00                     | 0.44              |
| 1:D:113:PRO:HA   | 1:D:116:LEU:HD12 | 1.99                     | 0.44              |
| 1:E:230:ILE:HG22 | 1:E:234:LEU:HG   | 1.99                     | 0.44              |
| 1:J:142:LYS:HD3  | 1:J:142:LYS:HA   | 1.72                     | 0.44              |
| 1:J:180:GLY:HA2  | 1:J:380:LYS:HD2  | 1.99                     | 0.44              |
| 1:K:513:LEU:HD23 | 1:K:513:LEU:HA   | 1.73                     | 0.44              |
| 1:G:195:PHE:HD2  | 1:G:197:ARG:HB2  | 1.82                     | 0.44              |
| 1:A:350:ARG:HA   | 1:A:353:ILE:HD13 | 1.99                     | 0.44              |
| 1:D:151:SER:HB3  | 1:D:399:ALA:HA   | 1.98                     | 0.44              |
| 1:E:383:ALA:HB3  | 1:E:389:MET:HE2  | 2.00                     | 0.44              |
| 1:F:248:LEU:HD22 | 1:F:323:VAL:HG11 | 2.00                     | 0.44              |
| 1:J:421:ARG:NH2  | 1:J:476:TYR:O    | 2.51                     | 0.44              |
| 1:K:230:ILE:O    | 1:K:233:MET:HE3  | 2.17                     | 0.44              |
| 1:M:441:LYS:HA   | 1:M:441:LYS:HD3  | 1.77                     | 0.44              |
| 1:B:478:TYR:OH   | 1:B:483:GLU:OE1  | 2.23                     | 0.44              |
| 1:C:356:ALA:O    | 1:C:362:ARG:NH2  | 2.49                     | 0.44              |
| 1:D:428:ASP:OD1  | 1:D:428:ASP:N    | 2.46                     | 0.44              |
| 1:F:267:MET:HB3  | 1:I:257:GLU:HA   | 2.00                     | 0.44              |
| 1:F:293:ALA:O    | 1:F:298:GLY:N    | 2.50                     | 0.44              |
| 1:H:419:LEU:HA   | 1:H:422:VAL:HG22 | 2.00                     | 0.44              |
| 1:G:456:LEU:HG   | 1:G:462:PRO:HG3  | 1.98                     | 0.43              |
| 1:A:290:GLN:NE2  | 1:A:291:ASP:OD1  | 2.50                     | 0.43              |
| 1:B:290:GLN:NE2  | 1:B:291:ASP:OD1  | 2.51                     | 0.43              |
| 1:C:498:LYS:HG3  | 1:C:501:ARG:HH21 | 1.83                     | 0.43              |
| 1:E:255:GLU:HG2  | 1:H:244:GLY:HA2  | 2.00                     | 0.43              |
| 1:F:290:GLN:NE2  | 1:F:291:ASP:OD1  | 2.51                     | 0.43              |
| 1:H:176:THR:HG21 | 1:H:333:ILE:HD11 | 1.99                     | 0.43              |
| 1:J:253:ASP:HB3  | 1:L:244:GLY:HA3  | 2.00                     | 0.43              |
| 1:L:40:LEU:HD13  | 1:L:59:GLU:HG3   | 2.00                     | 0.43              |
| 1:N:479:ASN:HB2  | 1:N:491:MET:CE   | 2.48                     | 0.43              |
| 1:G:227:ILE:HG21 | 1:G:232:GLU:HG3  | 2.00                     | 0.43              |
| 1:B:19:GLY:HA3   | 1:B:67:GLU:O     | 2.19                     | 0.43              |
| 1:C:69:MET:SD    | 1:C:522:THR:HB   | 2.58                     | 0.43              |
| 1:C:513:LEU:HD12 | 1:C:513:LEU:HA   | 1.70                     | 0.43              |
| 1:E:513:LEU:HD23 | 1:E:513:LEU:HA   | 1.73                     | 0.43              |
| 1:J:362:ARG:O    | 1:J:366:GLN:NE2  | 2.46                     | 0.43              |
| 1:K:69:MET:HE3   | 1:K:520:MET:HE2  | 1.99                     | 0.43              |
| 1:K:73:MET:O     | 1:K:76:GLU:HB3   | 2.18                     | 0.43              |
| 1:K:288:MET:SD   | 1:K:288:MET:N    | 2.91                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:151:SER:HB3  | 1:L:399:ALA:HA   | 1.98                     | 0.43              |
| 1:A:218:PRO:HA   | 1:A:246:PRO:HD2  | 2.00                     | 0.43              |
| 1:B:498:LYS:HG3  | 1:B:501:ARG:HH21 | 1.82                     | 0.43              |
| 1:D:231:ARG:HD3  | 1:D:234:LEU:HD12 | 1.99                     | 0.43              |
| 1:E:350:ARG:HA   | 1:E:353:ILE:HD12 | 2.00                     | 0.43              |
| 1:K:262:LEU:O    | 1:K:266:THR:OG1  | 2.31                     | 0.43              |
| 1:K:419:LEU:HA   | 1:K:422:VAL:HG22 | 2.00                     | 0.43              |
| 1:L:239:ALA:HB1  | 1:L:314:LEU:HD21 | 1.99                     | 0.43              |
| 1:M:390:LYS:HE3  | 5:M:757:HOH:O    | 2.19                     | 0.43              |
| 1:G:19:GLY:HA3   | 1:G:67:GLU:O     | 2.18                     | 0.43              |
| 1:D:142:LYS:HA   | 1:D:142:LYS:HD2  | 1.65                     | 0.43              |
| 1:D:422:VAL:HG23 | 1:D:447:MET:HE3  | 2.00                     | 0.43              |
| 1:E:151:SER:HB3  | 1:E:399:ALA:HA   | 1.99                     | 0.43              |
| 1:J:353:ILE:HG12 | 1:J:365:LEU:HB3  | 2.00                     | 0.43              |
| 1:L:13:ARG:HD2   | 1:L:104:LEU:HD22 | 2.01                     | 0.43              |
| 1:N:142:LYS:HD2  | 1:N:142:LYS:HA   | 1.63                     | 0.43              |
| 1:N:293:ALA:O    | 1:N:298:GLY:N    | 2.51                     | 0.43              |
| 1:N:510:VAL:O    | 1:N:514:MET:HG3  | 2.18                     | 0.43              |
| 1:G:176:THR:HG21 | 1:G:333:ILE:HD11 | 1.99                     | 0.43              |
| 1:B:61:GLU:O     | 1:D:4:LYS:N      | 2.46                     | 0.43              |
| 1:C:219:PHE:CD1  | 1:C:245:LYS:HD2  | 2.53                     | 0.43              |
| 1:F:19:GLY:HA3   | 1:F:67:GLU:O     | 2.19                     | 0.43              |
| 1:H:16:MET:HE2   | 1:H:16:MET:HB3   | 1.82                     | 0.43              |
| 1:K:42:LYS:HA    | 1:K:42:LYS:HD3   | 1.78                     | 0.43              |
| 1:N:262:LEU:O    | 1:N:266:THR:OG1  | 2.34                     | 0.43              |
| 1:A:23:LEU:HD11  | 1:A:75:LYS:HB2   | 2.00                     | 0.43              |
| 1:C:85:ALA:HB1   | 1:C:499:VAL:HG22 | 2.01                     | 0.43              |
| 1:C:195:PHE:CD2  | 1:C:197:ARG:HB2  | 2.53                     | 0.43              |
| 1:I:366:GLN:HA   | 1:I:369:VAL:HG22 | 2.01                     | 0.43              |
| 1:J:19:GLY:HA3   | 1:J:67:GLU:O     | 2.19                     | 0.43              |
| 1:K:290:GLN:NE2  | 1:K:291:ASP:OD1  | 2.51                     | 0.43              |
| 1:N:239:ALA:HB1  | 1:N:314:LEU:HD21 | 2.00                     | 0.43              |
| 1:G:325:ILE:HA   | 1:G:330:THR:HG23 | 2.00                     | 0.43              |
| 1:G:441:LYS:HA   | 1:G:441:LYS:HD3  | 1.78                     | 0.43              |
| 1:A:233:MET:HE1  | 1:C:242:LYS:HE2  | 1.99                     | 0.43              |
| 1:A:441:LYS:HA   | 1:A:441:LYS:HD3  | 1.79                     | 0.43              |
| 1:C:195:PHE:HB2  | 1:C:279:PRO:HG3  | 2.00                     | 0.43              |
| 1:C:221:LEU:HD23 | 1:C:249:ILE:HG12 | 2.01                     | 0.43              |
| 1:E:456:LEU:HG   | 1:E:462:PRO:HG3  | 2.00                     | 0.43              |
| 1:J:128:VAL:HG22 | 1:J:501:ARG:HG3  | 2.01                     | 0.43              |
| 1:J:254:VAL:HG21 | 1:J:275:ALA:HB1  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:255:GLU:HG2  | 1:L:244:GLY:HA2  | 2.00                     | 0.43              |
| 1:K:177:VAL:HG23 | 1:K:400:LEU:HD22 | 2.01                     | 0.43              |
| 1:L:27:VAL:O     | 1:L:30:THR:OG1   | 2.26                     | 0.43              |
| 1:L:322:ARG:HB3  | 1:L:333:ILE:HB   | 2.01                     | 0.43              |
| 1:M:419:LEU:HA   | 1:M:422:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:279:PRO:HG2  | 1:A:288:MET:HG3  | 2.01                     | 0.43              |
| 1:B:293:ALA:O    | 1:B:298:GLY:N    | 2.52                     | 0.43              |
| 1:C:197:ARG:HA   | 1:C:197:ARG:HD3  | 1.83                     | 0.43              |
| 1:D:207:LYS:HA   | 1:D:207:LYS:HD2  | 1.86                     | 0.43              |
| 1:D:236:VAL:HG21 | 1:D:309:LEU:HB3  | 2.01                     | 0.43              |
| 1:E:227:ILE:H    | 1:E:227:ILE:HG13 | 1.64                     | 0.43              |
| 1:F:421:ARG:NH2  | 1:F:476:TYR:O    | 2.52                     | 0.43              |
| 1:H:513:LEU:HD23 | 1:H:513:LEU:HA   | 1.77                     | 0.43              |
| 1:K:59:GLU:O     | 1:M:4:LYS:HG3    | 2.19                     | 0.43              |
| 1:M:85:ALA:HB1   | 1:M:499:VAL:HG22 | 2.01                     | 0.43              |
| 1:M:338:GLU:N    | 5:M:701:HOH:O    | 2.50                     | 0.43              |
| 1:N:128:VAL:O    | 1:N:132:LYS:HG2  | 2.18                     | 0.43              |
| 1:G:244:GLY:CA   | 1:B:255:GLU:HG2  | 2.48                     | 0.43              |
| 1:A:353:ILE:HG23 | 1:A:362:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:456:LEU:HG   | 1:A:462:PRO:HG3  | 1.99                     | 0.43              |
| 1:C:169:VAL:HG11 | 1:C:377:ALA:HB2  | 2.01                     | 0.43              |
| 1:C:201:SER:HB3  | 1:C:204:PHE:CD2  | 2.54                     | 0.43              |
| 1:H:128:VAL:O    | 1:H:132:LYS:HG2  | 2.18                     | 0.43              |
| 1:H:185:ASP:OD1  | 1:H:185:ASP:N    | 2.51                     | 0.43              |
| 1:H:365:LEU:O    | 1:H:369:VAL:HG22 | 2.18                     | 0.43              |
| 1:I:290:GLN:NE2  | 1:I:291:ASP:OD1  | 2.51                     | 0.43              |
| 1:K:126:ALA:O    | 1:K:130:GLU:HG2  | 2.18                     | 0.43              |
| 1:K:218:PRO:HG2  | 1:K:320:ALA:HB3  | 2.01                     | 0.43              |
| 1:K:383:ALA:HB3  | 1:K:389:MET:HE2  | 2.01                     | 0.43              |
| 1:G:23:LEU:HD11  | 1:G:75:LYS:HB2   | 2.01                     | 0.43              |
| 1:B:128:VAL:O    | 1:B:132:LYS:HG2  | 2.18                     | 0.43              |
| 1:B:218:PRO:HG2  | 1:B:320:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:421:ARG:NH2  | 1:B:476:TYR:O    | 2.51                     | 0.43              |
| 1:C:40:LEU:HD13  | 1:C:59:GLU:HG3   | 2.01                     | 0.43              |
| 1:C:441:LYS:HA   | 1:C:441:LYS:HD3  | 1.78                     | 0.43              |
| 1:D:100:ILE:HG13 | 1:D:511:ALA:HB1  | 2.00                     | 0.43              |
| 1:E:33:PRO:O     | 5:E:702:HOH:O    | 2.22                     | 0.43              |
| 1:H:177:VAL:HG23 | 1:H:400:LEU:HD22 | 2.01                     | 0.43              |
| 1:I:28:LYS:HD3   | 1:I:453:GLN:CD   | 2.44                     | 0.43              |
| 1:M:73:MET:HB3   | 1:M:514:MET:SD   | 2.59                     | 0.43              |
| 1:M:113:PRO:HA   | 1:M:116:LEU:HD12 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:421:ARG:NH2  | 1:M:476:TYR:O    | 2.51                     | 0.43              |
| 1:F:61:GLU:O     | 1:I:4:LYS:N      | 2.44                     | 0.42              |
| 1:H:441:LYS:HA   | 1:H:441:LYS:HD3  | 1.78                     | 0.42              |
| 1:K:201:SER:HB3  | 1:K:204:PHE:CD2  | 2.54                     | 0.42              |
| 1:M:290:GLN:NE2  | 1:M:291:ASP:OD1  | 2.52                     | 0.42              |
| 1:N:31:LEU:HD23  | 1:N:453:GLN:HB3  | 2.01                     | 0.42              |
| 1:N:350:ARG:HA   | 1:N:353:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:19:GLY:HA3   | 1:A:67:GLU:O     | 2.19                     | 0.42              |
| 1:A:353:ILE:HG23 | 1:A:362:ARG:CZ   | 2.49                     | 0.42              |
| 1:D:85:ALA:HB1   | 1:D:499:VAL:HG22 | 2.01                     | 0.42              |
| 1:E:498:LYS:HG3  | 1:E:501:ARG:HH21 | 1.85                     | 0.42              |
| 1:H:28:LYS:HD3   | 1:H:453:GLN:CD   | 2.44                     | 0.42              |
| 1:I:267:MET:HA   | 1:K:261:THR:HG21 | 2.00                     | 0.42              |
| 1:K:226:LYS:HD2  | 1:K:226:LYS:HA   | 1.72                     | 0.42              |
| 1:K:353:ILE:HG13 | 1:K:365:LEU:HB3  | 2.00                     | 0.42              |
| 1:G:70:GLY:HA2   | 1:G:73:MET:HE3   | 2.01                     | 0.42              |
| 1:G:256:GLY:HA3  | 1:M:270:ILE:HG21 | 2.01                     | 0.42              |
| 1:F:128:VAL:HG22 | 1:F:501:ARG:HG3  | 2.01                     | 0.42              |
| 1:H:174:VAL:HG13 | 1:H:376:VAL:HA   | 2.01                     | 0.42              |
| 1:I:422:VAL:HG23 | 1:I:447:MET:HE3  | 2.02                     | 0.42              |
| 1:I:441:LYS:HA   | 1:I:441:LYS:HD3  | 1.78                     | 0.42              |
| 1:K:349:ILE:HG23 | 1:K:365:LEU:HD22 | 2.01                     | 0.42              |
| 1:K:487:ASN:HB3  | 1:K:490:ASP:HB2  | 2.01                     | 0.42              |
| 1:L:111:MET:SD   | 1:L:438:VAL:HG21 | 2.59                     | 0.42              |
| 1:L:213:VAL:HG22 | 1:L:325:ILE:HB   | 2.00                     | 0.42              |
| 1:L:356:ALA:O    | 1:L:362:ARG:NH2  | 2.48                     | 0.42              |
| 1:M:128:VAL:O    | 1:M:132:LYS:HG2  | 2.19                     | 0.42              |
| 1:A:40:LEU:HD13  | 1:A:59:GLU:HG3   | 2.01                     | 0.42              |
| 1:A:128:VAL:O    | 1:A:132:LYS:HG2  | 2.18                     | 0.42              |
| 1:B:31:LEU:HD23  | 1:B:453:GLN:HB3  | 2.02                     | 0.42              |
| 1:B:363:GLU:O    | 1:B:366:GLN:HG2  | 2.20                     | 0.42              |
| 1:C:44:PHE:CD2   | 1:C:207:LYS:HE2  | 2.54                     | 0.42              |
| 1:C:263:VAL:O    | 1:C:267:MET:HG3  | 2.19                     | 0.42              |
| 1:D:325:ILE:HA   | 1:D:330:THR:HG23 | 2.00                     | 0.42              |
| 1:E:261:THR:HG21 | 1:H:267:MET:HA   | 2.01                     | 0.42              |
| 1:H:321:LYS:N    | 1:H:334:ASP:O    | 2.43                     | 0.42              |
| 1:J:160:LYS:HE3  | 1:J:160:LYS:HB3  | 1.84                     | 0.42              |
| 1:J:185:ASP:OD1  | 1:J:185:ASP:N    | 2.52                     | 0.42              |
| 1:M:323:VAL:HG12 | 1:M:332:ILE:HA   | 2.01                     | 0.42              |
| 1:N:197:ARG:HD3  | 1:N:197:ARG:HA   | 1.81                     | 0.42              |
| 1:C:325:ILE:HA   | 1:C:330:THR:HG23 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:421:ARG:NH2  | 1:C:476:TYR:O    | 2.51                     | 0.42              |
| 1:I:19:GLY:HA3   | 1:I:67:GLU:O     | 2.20                     | 0.42              |
| 1:L:85:ALA:HB1   | 1:L:499:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:197:ARG:HA   | 1:A:197:ARG:HD3  | 1.89                     | 0.42              |
| 1:A:419:LEU:HA   | 1:A:422:VAL:HG22 | 2.00                     | 0.42              |
| 1:B:365:LEU:HD23 | 1:B:365:LEU:HA   | 1.89                     | 0.42              |
| 1:D:243:ALA:O    | 1:F:253:ASP:HB3  | 2.20                     | 0.42              |
| 1:H:19:GLY:HA3   | 1:H:67:GLU:O     | 2.19                     | 0.42              |
| 1:J:213:VAL:HG23 | 1:J:325:ILE:HB   | 2.00                     | 0.42              |
| 1:M:226:LYS:HZ1  | 1:M:252:GLU:H    | 1.67                     | 0.42              |
| 1:A:361:ASP:HA   | 1:A:364:LYS:HE3  | 2.01                     | 0.42              |
| 1:B:383:ALA:HB3  | 1:B:389:MET:HE2  | 2.01                     | 0.42              |
| 1:C:113:PRO:HA   | 1:C:116:LEU:HD12 | 2.01                     | 0.42              |
| 1:D:244:GLY:HA3  | 1:F:253:ASP:HB3  | 2.02                     | 0.42              |
| 1:E:447:MET:HE2  | 1:E:504:LEU:HD21 | 2.02                     | 0.42              |
| 1:F:31:LEU:O     | 1:F:457:ASN:ND2  | 2.39                     | 0.42              |
| 1:L:111:MET:HG2  | 1:L:435:ASP:OD1  | 2.20                     | 0.42              |
| 1:L:320:ALA:HA   | 1:L:335:GLY:HA2  | 2.02                     | 0.42              |
| 1:G:28:LYS:C     | 1:G:30:THR:H     | 2.27                     | 0.42              |
| 1:A:233:MET:H    | 1:A:233:MET:HG2  | 1.63                     | 0.42              |
| 1:C:102:GLU:HB3  | 1:C:442:VAL:HG22 | 2.01                     | 0.42              |
| 1:C:207:LYS:HA   | 1:C:207:LYS:HD2  | 1.90                     | 0.42              |
| 1:H:288:MET:HE1  | 1:H:368:ARG:HD2  | 2.01                     | 0.42              |
| 1:K:365:LEU:HD23 | 1:K:365:LEU:HA   | 1.90                     | 0.42              |
| 1:L:7:LYS:HG3    | 1:L:66:PHE:CZ    | 2.55                     | 0.42              |
| 1:N:219:PHE:CD1  | 1:N:245:LYS:HD2  | 2.55                     | 0.42              |
| 1:N:421:ARG:NH2  | 1:N:476:TYR:O    | 2.52                     | 0.42              |
| 1:G:498:LYS:HG3  | 1:G:501:ARG:HH21 | 1.83                     | 0.42              |
| 1:A:498:LYS:HG3  | 1:A:501:ARG:HH21 | 1.84                     | 0.42              |
| 1:C:195:PHE:HD2  | 1:C:197:ARG:HB2  | 1.85                     | 0.42              |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HD22 | 2.02                     | 0.42              |
| 1:C:362:ARG:HH12 | 1:C:365:LEU:HD12 | 1.85                     | 0.42              |
| 1:D:42:LYS:HA    | 1:D:42:LYS:HD3   | 1.89                     | 0.42              |
| 1:F:42:LYS:HD3   | 1:F:42:LYS:HA    | 1.83                     | 0.42              |
| 1:I:247:LEU:HB3  | 1:I:273:VAL:HG22 | 2.02                     | 0.42              |
| 1:J:361:ASP:HA   | 1:J:364:LYS:HE3  | 2.01                     | 0.42              |
| 1:G:238:GLU:HB3  | 1:B:228:SER:O    | 2.19                     | 0.42              |
| 1:G:419:LEU:HA   | 1:G:422:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:186:GLU:HB2  | 1:A:380:LYS:HB2  | 2.01                     | 0.42              |
| 1:C:200:LEU:HD21 | 1:C:277:LYS:HG3  | 2.01                     | 0.42              |
| 1:D:365:LEU:O    | 1:D:369:VAL:HG22 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:180:GLY:HA2  | 1:F:380:LYS:HD2  | 2.00                     | 0.42              |
| 1:H:195:PHE:CD2  | 1:H:197:ARG:HB2  | 2.55                     | 0.42              |
| 1:H:290:GLN:NE2  | 1:H:291:ASP:OD1  | 2.53                     | 0.42              |
| 1:H:372:LEU:HD23 | 1:H:372:LEU:HA   | 1.87                     | 0.42              |
| 1:I:215:LEU:HB2  | 1:I:323:VAL:HG22 | 2.02                     | 0.42              |
| 1:J:293:ALA:O    | 1:J:298:GLY:N    | 2.50                     | 0.42              |
| 1:L:126:ALA:O    | 1:L:130:GLU:HG2  | 2.20                     | 0.42              |
| 1:L:206:ASN:H    | 1:L:213:VAL:HG12 | 1.85                     | 0.42              |
| 1:B:118:ARG:NH2  | 5:B:721:HOH:O    | 2.53                     | 0.41              |
| 1:C:349:ILE:HG23 | 1:C:365:LEU:HD22 | 2.01                     | 0.41              |
| 1:E:233:MET:HA   | 1:E:236:VAL:HG23 | 2.02                     | 0.41              |
| 1:E:419:LEU:HA   | 1:E:422:VAL:HG22 | 2.01                     | 0.41              |
| 1:E:487:ASN:HB3  | 1:E:490:ASP:HB2  | 2.02                     | 0.41              |
| 1:F:323:VAL:HG22 | 1:F:332:ILE:HA   | 2.02                     | 0.41              |
| 1:H:4:LYS:N      | 1:J:61:GLU:O     | 2.44                     | 0.41              |
| 1:K:193:MET:HE1  | 1:K:371:LYS:HD3  | 2.01                     | 0.41              |
| 1:K:241:ALA:O    | 1:M:255:GLU:HB2  | 2.19                     | 0.41              |
| 1:K:498:LYS:HG3  | 1:K:501:ARG:HH21 | 1.85                     | 0.41              |
| 1:N:69:MET:SD    | 1:N:522:THR:HB   | 2.60                     | 0.41              |
| 1:N:215:LEU:HD12 | 1:N:323:VAL:HB   | 2.00                     | 0.41              |
| 1:G:128:VAL:O    | 1:G:132:LYS:HG2  | 2.19                     | 0.41              |
| 1:C:100:ILE:CD1  | 1:C:514:MET:HB2  | 2.50                     | 0.41              |
| 1:C:440:ILE:O    | 1:C:444:LEU:HG   | 2.19                     | 0.41              |
| 1:D:392:LYS:O    | 1:D:396:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:293:ALA:O    | 1:E:298:GLY:N    | 2.53                     | 0.41              |
| 1:L:321:LYS:N    | 1:L:334:ASP:O    | 2.44                     | 0.41              |
| 1:N:261:THR:HA   | 1:N:264:VAL:HG12 | 2.02                     | 0.41              |
| 1:N:441:LYS:HD3  | 1:N:441:LYS:HA   | 1.78                     | 0.41              |
| 1:A:264:VAL:HG11 | 1:C:268:ARG:HH11 | 1.85                     | 0.41              |
| 1:C:112:ASN:ND2  | 5:C:715:HOH:O    | 2.44                     | 0.41              |
| 1:D:13:ARG:HD2   | 1:D:104:LEU:HD22 | 2.03                     | 0.41              |
| 1:F:158:VAL:O    | 1:F:162:ILE:HG13 | 2.20                     | 0.41              |
| 1:H:100:ILE:HG13 | 1:H:511:ALA:HB1  | 2.02                     | 0.41              |
| 1:I:195:PHE:HD2  | 1:I:197:ARG:HB2  | 1.85                     | 0.41              |
| 1:I:293:ALA:O    | 1:I:298:GLY:N    | 2.50                     | 0.41              |
| 1:J:201:SER:HB3  | 1:J:204:PHE:CD2  | 2.55                     | 0.41              |
| 1:J:206:ASN:HB3  | 1:J:208:PRO:HD2  | 2.01                     | 0.41              |
| 1:L:365:LEU:O    | 1:L:369:VAL:HG13 | 2.20                     | 0.41              |
| 1:N:201:SER:HB3  | 1:N:204:PHE:CD2  | 2.54                     | 0.41              |
| 1:G:293:ALA:O    | 1:G:298:GLY:N    | 2.53                     | 0.41              |
| 1:B:387:VAL:HG13 | 1:D:513:LEU:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:135:SER:HB2  | 1:D:497:THR:HG21 | 2.02                     | 0.41              |
| 1:E:234:LEU:HA   | 1:E:234:LEU:HD23 | 1.89                     | 0.41              |
| 1:E:362:ARG:HA   | 1:E:362:ARG:NE   | 2.35                     | 0.41              |
| 1:E:510:VAL:HG23 | 1:H:385:THR:HG21 | 2.02                     | 0.41              |
| 1:I:80:LYS:HA    | 1:I:80:LYS:HD2   | 1.96                     | 0.41              |
| 1:I:128:VAL:O    | 1:I:132:LYS:HG2  | 2.20                     | 0.41              |
| 1:I:201:SER:HB3  | 1:I:204:PHE:CD2  | 2.55                     | 0.41              |
| 1:K:19:GLY:HA3   | 1:K:67:GLU:O     | 2.20                     | 0.41              |
| 1:K:176:THR:HG21 | 1:K:333:ILE:HD11 | 2.02                     | 0.41              |
| 1:L:226:LYS:NZ   | 1:L:253:ASP:O    | 2.38                     | 0.41              |
| 1:L:513:LEU:HA   | 1:L:513:LEU:HD23 | 1.72                     | 0.41              |
| 1:M:73:MET:O     | 1:M:76:GLU:HB3   | 2.19                     | 0.41              |
| 1:N:247:LEU:HB3  | 1:N:273:VAL:HG13 | 2.02                     | 0.41              |
| 1:N:325:ILE:HA   | 1:N:330:THR:HG23 | 2.02                     | 0.41              |
| 1:N:419:LEU:HA   | 1:N:422:VAL:HG22 | 2.01                     | 0.41              |
| 1:N:456:LEU:HG   | 1:N:462:PRO:HG3  | 2.01                     | 0.41              |
| 1:G:228:SER:HA   | 1:M:239:ALA:HA   | 2.02                     | 0.41              |
| 1:A:73:MET:O     | 1:A:76:GLU:HB3   | 2.21                     | 0.41              |
| 1:B:135:SER:O    | 5:B:701:HOH:O    | 2.22                     | 0.41              |
| 1:B:390:LYS:HE3  | 5:B:756:HOH:O    | 2.20                     | 0.41              |
| 1:D:206:ASN:HB3  | 1:D:208:PRO:HD2  | 2.02                     | 0.41              |
| 1:H:422:VAL:HG23 | 1:H:447:MET:HE3  | 2.02                     | 0.41              |
| 1:J:124:VAL:HG13 | 1:J:504:LEU:HG   | 2.02                     | 0.41              |
| 1:J:219:PHE:CD1  | 1:J:245:LYS:HD2  | 2.55                     | 0.41              |
| 1:J:239:ALA:HB1  | 1:J:314:LEU:HD21 | 2.01                     | 0.41              |
| 1:L:207:LYS:NZ   | 5:L:714:HOH:O    | 2.47                     | 0.41              |
| 1:L:278:ALA:HB3  | 1:L:285:ARG:HH11 | 1.85                     | 0.41              |
| 1:N:361:ASP:HA   | 1:N:364:LYS:HG2  | 2.02                     | 0.41              |
| 1:G:16:MET:HE2   | 1:G:16:MET:HB3   | 1.89                     | 0.41              |
| 1:A:195:PHE:CD2  | 1:A:197:ARG:HB2  | 2.56                     | 0.41              |
| 1:A:230:ILE:HG23 | 1:C:238:GLU:OE1  | 2.21                     | 0.41              |
| 1:B:40:LEU:HD13  | 1:B:59:GLU:HG3   | 2.02                     | 0.41              |
| 1:C:307:MET:HE1  | 1:C:312:ALA:HB2  | 2.02                     | 0.41              |
| 1:D:193:MET:HA   | 1:D:193:MET:CE   | 2.43                     | 0.41              |
| 1:E:174:VAL:HG13 | 1:E:376:VAL:HA   | 2.03                     | 0.41              |
| 1:E:207:LYS:HA   | 1:E:207:LYS:HD2  | 1.95                     | 0.41              |
| 1:F:28:LYS:HD3   | 1:F:453:GLN:CD   | 2.46                     | 0.41              |
| 1:F:144:ILE:H    | 1:F:144:ILE:HG12 | 1.63                     | 0.41              |
| 1:F:390:LYS:HE3  | 5:F:740:HOH:O    | 2.20                     | 0.41              |
| 1:I:25:ASP:O     | 1:I:29:VAL:HG13  | 2.21                     | 0.41              |
| 1:I:478:TYR:OH   | 1:I:483:GLU:OE1  | 2.22                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:516:THR:OG1  | 1:L:37:ASN:ND2   | 2.43                     | 0.41              |
| 1:K:33:PRO:O     | 5:K:701:HOH:O    | 2.22                     | 0.41              |
| 1:K:232:GLU:OE2  | 1:K:233:MET:HG3  | 2.20                     | 0.41              |
| 1:L:102:GLU:HB3  | 1:L:442:VAL:HG22 | 2.02                     | 0.41              |
| 1:L:325:ILE:HA   | 1:L:330:THR:HG23 | 2.02                     | 0.41              |
| 1:L:382:GLY:O    | 1:L:392:LYS:NZ   | 2.40                     | 0.41              |
| 1:M:325:ILE:HA   | 1:M:330:THR:HG23 | 2.02                     | 0.41              |
| 1:M:440:ILE:O    | 1:M:444:LEU:HG   | 2.20                     | 0.41              |
| 1:G:73:MET:O     | 1:G:76:GLU:HB3   | 2.21                     | 0.41              |
| 1:G:226:LYS:HB2  | 1:G:226:LYS:HE3  | 1.85                     | 0.41              |
| 1:G:236:VAL:HG21 | 1:G:309:LEU:HB3  | 2.01                     | 0.41              |
| 1:A:180:GLY:HA2  | 1:A:380:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:362:ARG:NH2  | 1:A:366:GLN:OE1  | 2.54                     | 0.41              |
| 1:B:361:ASP:HA   | 1:B:364:LYS:HG2  | 2.02                     | 0.41              |
| 1:C:365:LEU:O    | 1:C:369:VAL:HG22 | 2.20                     | 0.41              |
| 1:E:353:ILE:CG2  | 1:E:366:GLN:HE22 | 2.33                     | 0.41              |
| 1:F:218:PRO:HG3  | 1:F:323:VAL:HB   | 2.03                     | 0.41              |
| 1:F:243:ALA:O    | 1:I:253:ASP:HB3  | 2.21                     | 0.41              |
| 1:H:293:ALA:O    | 1:H:298:GLY:N    | 2.53                     | 0.41              |
| 1:I:100:ILE:HG13 | 1:I:511:ALA:HB1  | 2.02                     | 0.41              |
| 1:I:452:ARG:NH2  | 1:I:463:SER:OG   | 2.54                     | 0.41              |
| 1:L:293:ALA:O    | 1:L:298:GLY:N    | 2.52                     | 0.41              |
| 1:L:419:LEU:HA   | 1:L:422:VAL:HG22 | 2.03                     | 0.41              |
| 1:G:216:GLU:OE1  | 1:G:216:GLU:N    | 2.54                     | 0.41              |
| 1:G:264:VAL:HG11 | 1:M:268:ARG:HH11 | 1.86                     | 0.41              |
| 1:G:362:ARG:HH12 | 1:G:365:LEU:HD12 | 1.86                     | 0.41              |
| 1:G:510:VAL:HG23 | 1:M:385:THR:HG21 | 2.02                     | 0.41              |
| 1:B:419:LEU:HA   | 1:B:422:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:390:LYS:HE3  | 5:C:758:HOH:O    | 2.21                     | 0.41              |
| 1:D:419:LEU:HA   | 1:D:422:VAL:HG22 | 2.03                     | 0.41              |
| 1:E:361:ASP:HA   | 1:E:364:LYS:HE3  | 2.02                     | 0.41              |
| 1:F:201:SER:HB3  | 1:F:204:PHE:CD2  | 2.55                     | 0.41              |
| 1:J:372:LEU:HD23 | 1:J:372:LEU:HA   | 1.84                     | 0.41              |
| 1:L:201:SER:HB3  | 1:L:204:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:102:GLU:HB3  | 1:A:442:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:257:GLU:HB3  | 1:C:271:VAL:HB   | 2.02                     | 0.41              |
| 1:A:293:ALA:O    | 1:A:298:GLY:N    | 2.53                     | 0.41              |
| 1:A:479:ASN:HB2  | 1:A:491:MET:CE   | 2.51                     | 0.41              |
| 1:C:54:VAL:HB    | 1:C:89:THR:HG21  | 2.02                     | 0.41              |
| 1:E:19:GLY:HA3   | 1:E:67:GLU:O     | 2.20                     | 0.41              |
| 1:E:128:VAL:O    | 1:E:132:LYS:HG2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:198:GLY:HA3  | 1:E:327:LYS:HA   | 2.02                     | 0.41              |
| 1:E:441:LYS:HA   | 1:E:441:LYS:HD3  | 1.79                     | 0.41              |
| 1:H:195:PHE:HB2  | 1:H:279:PRO:HG3  | 2.02                     | 0.41              |
| 1:H:226:LYS:HA   | 1:H:226:LYS:HD2  | 1.70                     | 0.41              |
| 1:H:230:ILE:HG23 | 1:H:231:ARG:HE   | 1.85                     | 0.41              |
| 1:I:216:GLU:HG3  | 1:I:322:ARG:HD2  | 2.03                     | 0.41              |
| 1:I:345:ARG:HD3  | 1:I:345:ARG:HA   | 1.85                     | 0.41              |
| 1:I:392:LYS:O    | 1:I:396:VAL:HG23 | 2.21                     | 0.41              |
| 1:J:28:LYS:HD3   | 1:J:453:GLN:CD   | 2.46                     | 0.41              |
| 1:J:236:VAL:HG21 | 1:J:309:LEU:HD22 | 2.03                     | 0.41              |
| 1:J:345:ARG:HD3  | 1:J:345:ARG:HA   | 1.89                     | 0.41              |
| 1:L:128:VAL:O    | 1:L:132:LYS:HG2  | 2.20                     | 0.41              |
| 1:L:195:PHE:CD2  | 1:L:197:ARG:HB2  | 2.56                     | 0.41              |
| 1:M:218:PRO:HD2  | 1:M:320:ALA:C    | 2.46                     | 0.41              |
| 1:M:349:ILE:O    | 1:M:353:ILE:HG13 | 2.21                     | 0.41              |
| 1:N:285:ARG:O    | 1:N:288:MET:HG2  | 2.21                     | 0.41              |
| 1:N:322:ARG:HB3  | 1:N:333:ILE:HB   | 2.02                     | 0.41              |
| 1:N:323:VAL:HG22 | 1:N:332:ILE:HA   | 2.03                     | 0.41              |
| 1:A:372:LEU:HD23 | 1:A:372:LEU:HA   | 1.85                     | 0.41              |
| 1:D:513:LEU:HA   | 1:D:513:LEU:HD23 | 1.72                     | 0.41              |
| 1:F:479:ASN:HB2  | 1:F:491:MET:SD   | 2.61                     | 0.41              |
| 1:K:28:LYS:HD3   | 1:K:453:GLN:CD   | 2.46                     | 0.41              |
| 1:L:100:ILE:HG13 | 1:L:511:ALA:HB1  | 2.01                     | 0.41              |
| 1:G:268:ARG:HH11 | 1:B:264:VAL:HG11 | 1.85                     | 0.40              |
| 1:B:456:LEU:HG   | 1:B:462:PRO:HG3  | 2.02                     | 0.40              |
| 1:C:39:VAL:HG22  | 1:C:49:ILE:HG12  | 2.03                     | 0.40              |
| 1:F:128:VAL:O    | 1:F:132:LYS:HG2  | 2.21                     | 0.40              |
| 1:H:233:MET:HG2  | 1:H:237:LEU:HD13 | 2.03                     | 0.40              |
| 1:H:322:ARG:HB3  | 1:H:333:ILE:HB   | 2.03                     | 0.40              |
| 1:I:219:PHE:HE2  | 1:I:314:LEU:HD22 | 1.86                     | 0.40              |
| 1:K:128:VAL:O    | 1:K:132:LYS:HG2  | 2.21                     | 0.40              |
| 1:L:197:ARG:HA   | 1:L:197:ARG:HD3  | 1.89                     | 0.40              |
| 1:N:230:ILE:HD13 | 1:N:230:ILE:HA   | 1.93                     | 0.40              |
| 1:G:237:LEU:HA   | 1:G:240:VAL:HG12 | 2.03                     | 0.40              |
| 1:A:27:VAL:O     | 1:A:30:THR:OG1   | 2.28                     | 0.40              |
| 1:B:239:ALA:HA   | 1:D:228:SER:HA   | 2.02                     | 0.40              |
| 1:D:111:MET:SD   | 1:D:438:VAL:HG21 | 2.60                     | 0.40              |
| 1:H:221:LEU:HD23 | 1:H:249:ILE:HG12 | 2.03                     | 0.40              |
| 1:I:267:MET:HG2  | 1:K:257:GLU:HB3  | 2.04                     | 0.40              |
| 1:K:218:PRO:HA   | 1:K:246:PRO:HG2  | 2.03                     | 0.40              |
| 1:K:390:LYS:HE3  | 5:K:756:HOH:O    | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:221:LEU:HD23 | 1:L:249:ILE:HG12 | 2.02                     | 0.40              |
| 1:M:174:VAL:HG21 | 1:M:194:GLN:HG3  | 2.03                     | 0.40              |
| 1:N:19:GLY:HA3   | 1:N:67:GLU:O     | 2.21                     | 0.40              |
| 1:G:225:LYS:HG2  | 1:G:302:SER:HA   | 2.04                     | 0.40              |
| 1:G:390:LYS:HE3  | 5:G:759:HOH:O    | 2.20                     | 0.40              |
| 1:A:201:SER:HB3  | 1:A:204:PHE:CD2  | 2.57                     | 0.40              |
| 1:B:254:VAL:HG11 | 1:B:259:LEU:HD23 | 2.03                     | 0.40              |
| 1:E:28:LYS:HD3   | 1:E:453:GLN:CD   | 2.46                     | 0.40              |
| 1:I:385:THR:HG21 | 1:K:510:VAL:HG23 | 2.03                     | 0.40              |
| 1:J:31:LEU:HD23  | 1:J:453:GLN:HB3  | 2.03                     | 0.40              |
| 1:N:39:VAL:HG22  | 1:N:49:ILE:HG12  | 2.03                     | 0.40              |
| 1:A:28:LYS:HD3   | 1:A:453:GLN:CD   | 2.46                     | 0.40              |
| 1:A:510:VAL:HG23 | 1:C:385:THR:HG21 | 2.02                     | 0.40              |
| 1:B:219:PHE:CD1  | 1:B:245:LYS:HD2  | 2.56                     | 0.40              |
| 1:B:411:VAL:HG21 | 1:B:494:LEU:HD23 | 2.03                     | 0.40              |
| 1:C:4:LYS:HG3    | 1:E:59:GLU:O     | 2.21                     | 0.40              |
| 1:C:100:ILE:HD11 | 1:C:511:ALA:HA   | 2.04                     | 0.40              |
| 1:E:102:GLU:HB3  | 1:E:442:VAL:HG22 | 2.03                     | 0.40              |
| 1:F:150:ILE:HD13 | 1:F:150:ILE:HA   | 1.87                     | 0.40              |
| 1:K:441:LYS:HA   | 1:K:441:LYS:HD3  | 1.80                     | 0.40              |
| 1:L:204:PHE:O    | 1:L:213:VAL:HG11 | 2.21                     | 0.40              |
| 1:G:218:PRO:HA   | 1:G:246:PRO:HG2  | 2.03                     | 0.40              |
| 1:B:365:LEU:O    | 1:B:369:VAL:HG13 | 2.21                     | 0.40              |
| 1:D:37:ASN:ND2   | 1:F:516:THR:OG1  | 2.44                     | 0.40              |
| 1:D:177:VAL:HG23 | 1:D:400:LEU:HD22 | 2.04                     | 0.40              |
| 1:E:169:VAL:HG11 | 1:E:377:ALA:HB2  | 2.04                     | 0.40              |
| 1:F:430:ARG:HD3  | 1:F:430:ARG:HA   | 1.93                     | 0.40              |
| 1:L:392:LYS:O    | 1:L:396:VAL:HG23 | 2.22                     | 0.40              |
| 1:M:39:VAL:HG22  | 1:M:49:ILE:HG12  | 2.04                     | 0.40              |
| 1:N:304:GLU:H    | 1:N:304:GLU:HG3  | 1.73                     | 0.40              |
| 1:N:320:ALA:HA   | 1:N:335:GLY:HA2  | 2.04                     | 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     | 522/548 (95%)   | 512 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 1   | B     | 522/548 (95%)   | 519 (99%)  | 2 (0%)  | 1 (0%)   | 43          | 68  |
| 1   | C     | 522/548 (95%)   | 517 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | D     | 522/548 (95%)   | 518 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | E     | 522/548 (95%)   | 518 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | F     | 522/548 (95%)   | 518 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | G     | 522/548 (95%)   | 517 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | H     | 522/548 (95%)   | 517 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | I     | 522/548 (95%)   | 518 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | J     | 522/548 (95%)   | 518 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | K     | 522/548 (95%)   | 521 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | L     | 522/548 (95%)   | 517 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | M     | 522/548 (95%)   | 515 (99%)  | 7 (1%)  | 0        | 100         | 100 |
| 1   | N     | 522/548 (95%)   | 517 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| All | All   | 7308/7672 (95%) | 7242 (99%) | 65 (1%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 253 | ASP  |

### 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     | 403/415 (97%) | 397 (98%) | 6 (2%)   | 57          | 81 |
| 1   | B     | 403/415 (97%) | 395 (98%) | 8 (2%)   | 48          | 76 |
| 1   | C     | 403/415 (97%) | 400 (99%) | 3 (1%)   | 76          | 90 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | D     | 403/415 (97%)   | 395 (98%)  | 8 (2%)   | 48          | 76 |
| 1   | E     | 403/415 (97%)   | 398 (99%)  | 5 (1%)   | 63          | 84 |
| 1   | F     | 403/415 (97%)   | 396 (98%)  | 7 (2%)   | 53          | 79 |
| 1   | G     | 403/415 (97%)   | 394 (98%)  | 9 (2%)   | 45          | 74 |
| 1   | H     | 403/415 (97%)   | 398 (99%)  | 5 (1%)   | 63          | 84 |
| 1   | I     | 403/415 (97%)   | 399 (99%)  | 4 (1%)   | 68          | 86 |
| 1   | J     | 403/415 (97%)   | 397 (98%)  | 6 (2%)   | 57          | 81 |
| 1   | K     | 403/415 (97%)   | 399 (99%)  | 4 (1%)   | 68          | 86 |
| 1   | L     | 403/415 (97%)   | 399 (99%)  | 4 (1%)   | 68          | 86 |
| 1   | M     | 403/415 (97%)   | 398 (99%)  | 5 (1%)   | 63          | 84 |
| 1   | N     | 403/415 (97%)   | 397 (98%)  | 6 (2%)   | 57          | 81 |
| All | All   | 5642/5810 (97%) | 5562 (99%) | 80 (1%)  | 57          | 82 |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 31  | LEU  |
| 1   | G     | 138 | CYS  |
| 1   | G     | 185 | ASP  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 236 | VAL  |
| 1   | G     | 262 | LEU  |
| 1   | G     | 376 | VAL  |
| 1   | G     | 502 | SER  |
| 1   | G     | 524 | LEU  |
| 1   | A     | 138 | CYS  |
| 1   | A     | 224 | ASP  |
| 1   | A     | 236 | VAL  |
| 1   | A     | 376 | VAL  |
| 1   | A     | 502 | SER  |
| 1   | A     | 524 | LEU  |
| 1   | B     | 138 | CYS  |
| 1   | B     | 142 | LYS  |
| 1   | B     | 262 | LEU  |
| 1   | B     | 289 | LEU  |
| 1   | B     | 358 | SER  |
| 1   | B     | 376 | VAL  |
| 1   | B     | 467 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 502 | SER  |
| 1   | C     | 138 | CYS  |
| 1   | C     | 142 | LYS  |
| 1   | C     | 502 | SER  |
| 1   | D     | 138 | CYS  |
| 1   | D     | 142 | LYS  |
| 1   | D     | 236 | VAL  |
| 1   | D     | 323 | VAL  |
| 1   | D     | 376 | VAL  |
| 1   | D     | 467 | ASN  |
| 1   | D     | 502 | SER  |
| 1   | D     | 513 | LEU  |
| 1   | E     | 138 | CYS  |
| 1   | E     | 236 | VAL  |
| 1   | E     | 366 | GLN  |
| 1   | E     | 369 | VAL  |
| 1   | E     | 502 | SER  |
| 1   | F     | 142 | LYS  |
| 1   | F     | 144 | ILE  |
| 1   | F     | 193 | MET  |
| 1   | F     | 236 | VAL  |
| 1   | F     | 323 | VAL  |
| 1   | F     | 376 | VAL  |
| 1   | F     | 502 | SER  |
| 1   | H     | 138 | CYS  |
| 1   | H     | 185 | ASP  |
| 1   | H     | 213 | VAL  |
| 1   | H     | 240 | VAL  |
| 1   | H     | 502 | SER  |
| 1   | I     | 138 | CYS  |
| 1   | I     | 142 | LYS  |
| 1   | I     | 264 | VAL  |
| 1   | I     | 502 | SER  |
| 1   | J     | 111 | MET  |
| 1   | J     | 138 | CYS  |
| 1   | J     | 366 | GLN  |
| 1   | J     | 376 | VAL  |
| 1   | J     | 428 | ASP  |
| 1   | J     | 502 | SER  |
| 1   | K     | 76  | GLU  |
| 1   | K     | 138 | CYS  |
| 1   | K     | 376 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 502 | SER  |
| 1   | L     | 138 | CYS  |
| 1   | L     | 376 | VAL  |
| 1   | L     | 467 | ASN  |
| 1   | L     | 502 | SER  |
| 1   | M     | 138 | CYS  |
| 1   | M     | 151 | SER  |
| 1   | M     | 230 | ILE  |
| 1   | M     | 262 | LEU  |
| 1   | M     | 502 | SER  |
| 1   | N     | 138 | CYS  |
| 1   | N     | 142 | LYS  |
| 1   | N     | 240 | VAL  |
| 1   | N     | 272 | LYS  |
| 1   | N     | 376 | VAL  |
| 1   | N     | 502 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 10  | ASN  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 487 | ASN  |
| 1   | A     | 10  | ASN  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 487 | ASN  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 206 | ASN  |
| 1   | D     | 37  | ASN  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 487 | ASN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 229 | ASN  |
| 1   | E     | 290 | GLN  |
| 1   | F     | 290 | GLN  |
| 1   | F     | 467 | ASN  |
| 1   | H     | 37  | ASN  |
| 1   | H     | 229 | ASN  |
| 1   | H     | 290 | GLN  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 290 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 37  | ASN  |
| 1   | J     | 290 | GLN  |
| 1   | K     | 82  | ASN  |
| 1   | K     | 290 | GLN  |
| 1   | L     | 290 | GLN  |
| 1   | L     | 487 | ASN  |
| 1   | M     | 229 | ASN  |
| 1   | M     | 290 | GLN  |
| 1   | N     | 290 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 28 are monoatomic - leaving 14 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | ATP  | A     | 602 | 2,4  | 32,33,33     | 0.70 | 1 (3%)      | 48,52,52    | 0.36 | 0           |
| 3   | ATP  | N     | 602 | 2,4  | 32,33,33     | 0.72 | 1 (3%)      | 48,52,52    | 0.37 | 0           |
| 3   | ATP  | M     | 602 | 2,4  | 32,33,33     | 0.75 | 1 (3%)      | 48,52,52    | 0.38 | 0           |
| 3   | ATP  | H     | 602 | 2,4  | 32,33,33     | 0.74 | 2 (6%)      | 48,52,52    | 0.37 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ATP  | G     | 602 | 2,4  | 32,33,33     | 0.69 | 1 (3%)   | 48,52,52    | 0.36 | 0        |
| 3   | ATP  | L     | 602 | 2,4  | 32,33,33     | 0.71 | 1 (3%)   | 48,52,52    | 0.36 | 0        |
| 3   | ATP  | D     | 602 | 2,4  | 32,33,33     | 0.69 | 1 (3%)   | 48,52,52    | 0.36 | 0        |
| 3   | ATP  | K     | 602 | 2,4  | 32,33,33     | 0.70 | 1 (3%)   | 48,52,52    | 0.35 | 0        |
| 3   | ATP  | I     | 602 | 2,4  | 32,33,33     | 0.74 | 2 (6%)   | 48,52,52    | 0.37 | 0        |
| 3   | ATP  | J     | 602 | 2,4  | 32,33,33     | 0.64 | 1 (3%)   | 48,52,52    | 0.36 | 0        |
| 3   | ATP  | E     | 602 | 2,4  | 32,33,33     | 0.69 | 1 (3%)   | 48,52,52    | 0.35 | 0        |
| 3   | ATP  | C     | 602 | 2,4  | 32,33,33     | 0.76 | 1 (3%)   | 48,52,52    | 0.38 | 0        |
| 3   | ATP  | F     | 602 | 2,4  | 32,33,33     | 0.63 | 1 (3%)   | 48,52,52    | 0.36 | 0        |
| 3   | ATP  | B     | 602 | 2,4  | 32,33,33     | 0.72 | 1 (3%)   | 48,52,52    | 0.37 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | ATP  | A     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | N     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | M     | 602 | 2,4  | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | ATP  | H     | 602 | 2,4  | -       | 2/22/38/38 | 0/3/3/3 |
| 3   | ATP  | G     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | L     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | D     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | K     | 602 | 2,4  | -       | 2/22/38/38 | 0/3/3/3 |
| 3   | ATP  | I     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | J     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | E     | 602 | 2,4  | -       | 2/22/38/38 | 0/3/3/3 |
| 3   | ATP  | C     | 602 | 2,4  | -       | 5/22/38/38 | 0/3/3/3 |
| 3   | ATP  | F     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | ATP  | B     | 602 | 2,4  | -       | 1/22/38/38 | 0/3/3/3 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 602 | ATP  | PA-O3A | -3.25 | 1.56        | 1.59     |
| 3   | C     | 602 | ATP  | PA-O3A | -3.24 | 1.56        | 1.59     |
| 3   | N     | 602 | ATP  | PA-O3A | -2.93 | 1.56        | 1.59     |
| 3   | B     | 602 | ATP  | PA-O3A | -2.91 | 1.56        | 1.59     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | L     | 602 | ATP  | PA-O3A | -2.86 | 1.56        | 1.59     |
| 3   | I     | 602 | ATP  | PA-O3A | -2.85 | 1.56        | 1.59     |
| 3   | D     | 602 | ATP  | PA-O3A | -2.84 | 1.56        | 1.59     |
| 3   | H     | 602 | ATP  | PA-O3A | -2.81 | 1.56        | 1.59     |
| 3   | A     | 602 | ATP  | PA-O3A | -2.73 | 1.56        | 1.59     |
| 3   | G     | 602 | ATP  | PA-O3A | -2.69 | 1.56        | 1.59     |
| 3   | K     | 602 | ATP  | PA-O3A | -2.65 | 1.56        | 1.59     |
| 3   | E     | 602 | ATP  | PA-O3A | -2.60 | 1.56        | 1.59     |
| 3   | J     | 602 | ATP  | PA-O3A | -2.22 | 1.57        | 1.59     |
| 3   | F     | 602 | ATP  | PA-O3A | -2.20 | 1.57        | 1.59     |
| 3   | I     | 602 | ATP  | PB-O3B | -2.08 | 1.57        | 1.59     |
| 3   | H     | 602 | ATP  | PB-O3B | -2.06 | 1.57        | 1.59     |

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

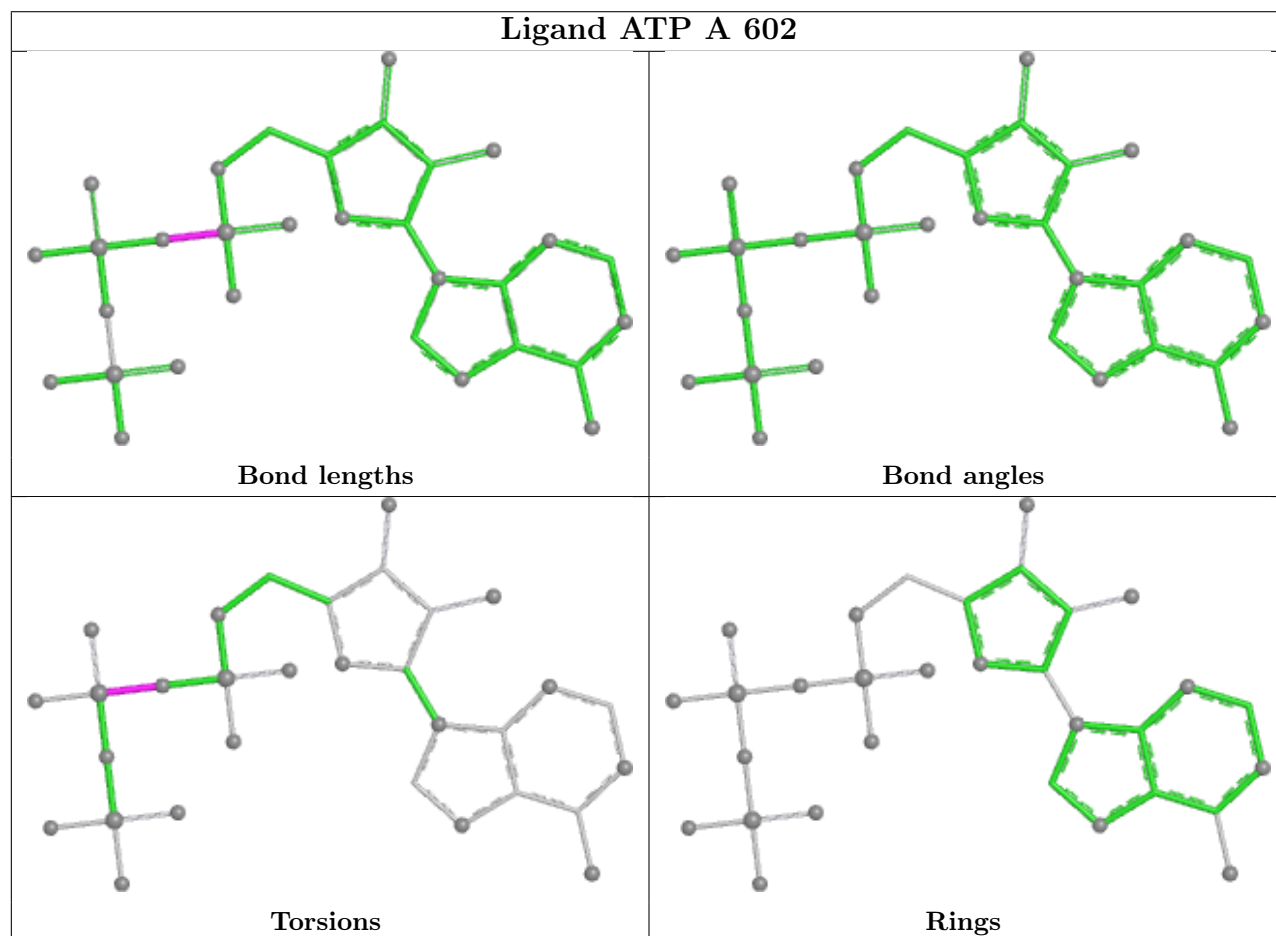
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 602 | ATP  | PB-O3B-PG-O2G   |
| 3   | C     | 602 | ATP  | PB-O3B-PG-O3G   |
| 3   | M     | 602 | ATP  | PB-O3B-PG-O2G   |
| 3   | M     | 602 | ATP  | PB-O3B-PG-O3G   |
| 3   | C     | 602 | ATP  | PB-O3A-PA-O1A   |
| 3   | M     | 602 | ATP  | PB-O3A-PA-O1A   |
| 3   | C     | 602 | ATP  | PB-O3A-PA-O2A   |
| 3   | M     | 602 | ATP  | PB-O3A-PA-O2A   |
| 3   | E     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 3   | K     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 3   | E     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | F     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | H     | 602 | ATP  | PA-O3A-PB-O1B   |
| 3   | H     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | I     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | J     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | K     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | G     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | A     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | B     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | C     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | D     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | L     | 602 | ATP  | PA-O3A-PB-O2B   |
| 3   | N     | 602 | ATP  | PA-O3A-PB-O2B   |

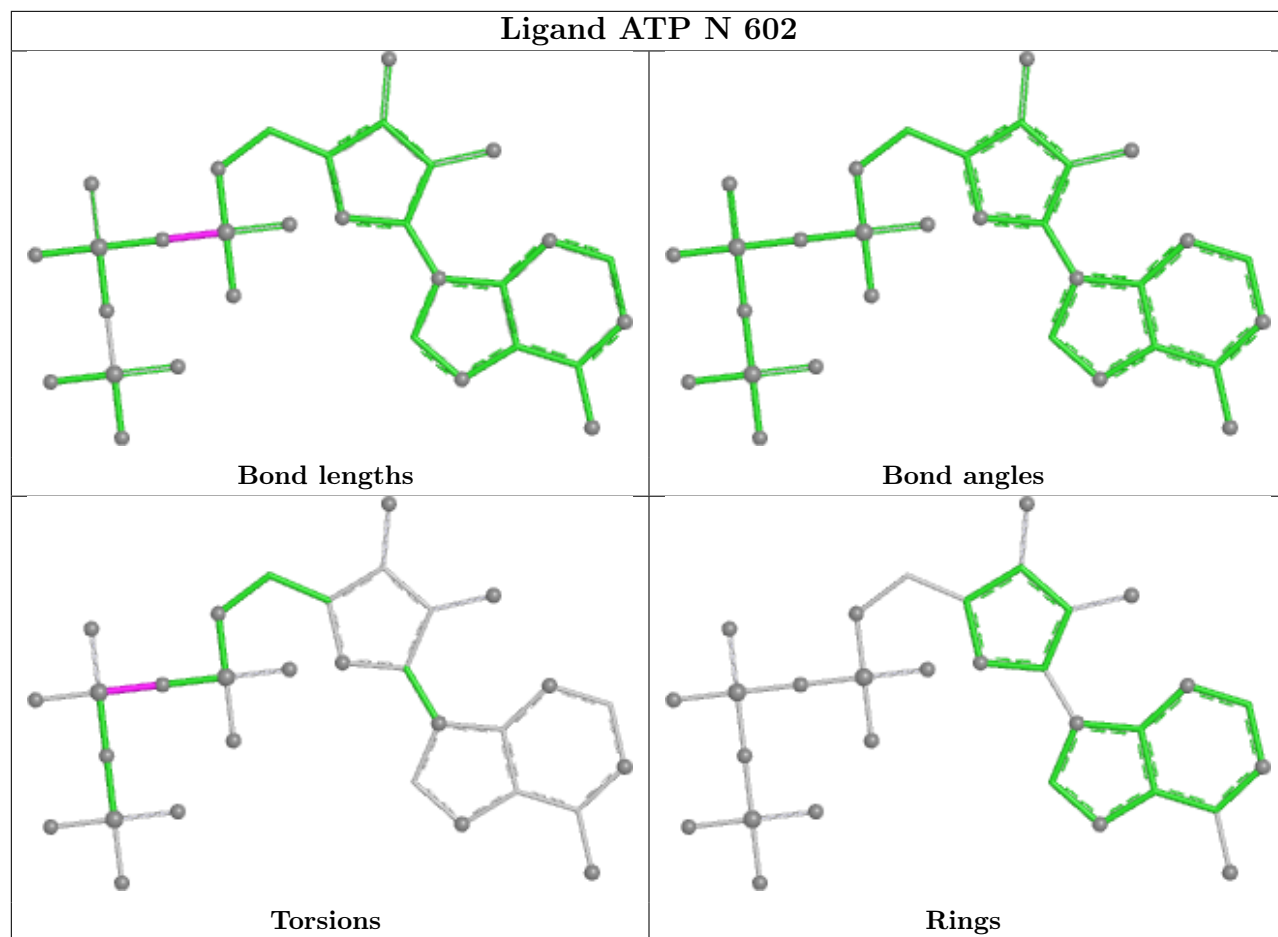
There are no ring outliers.

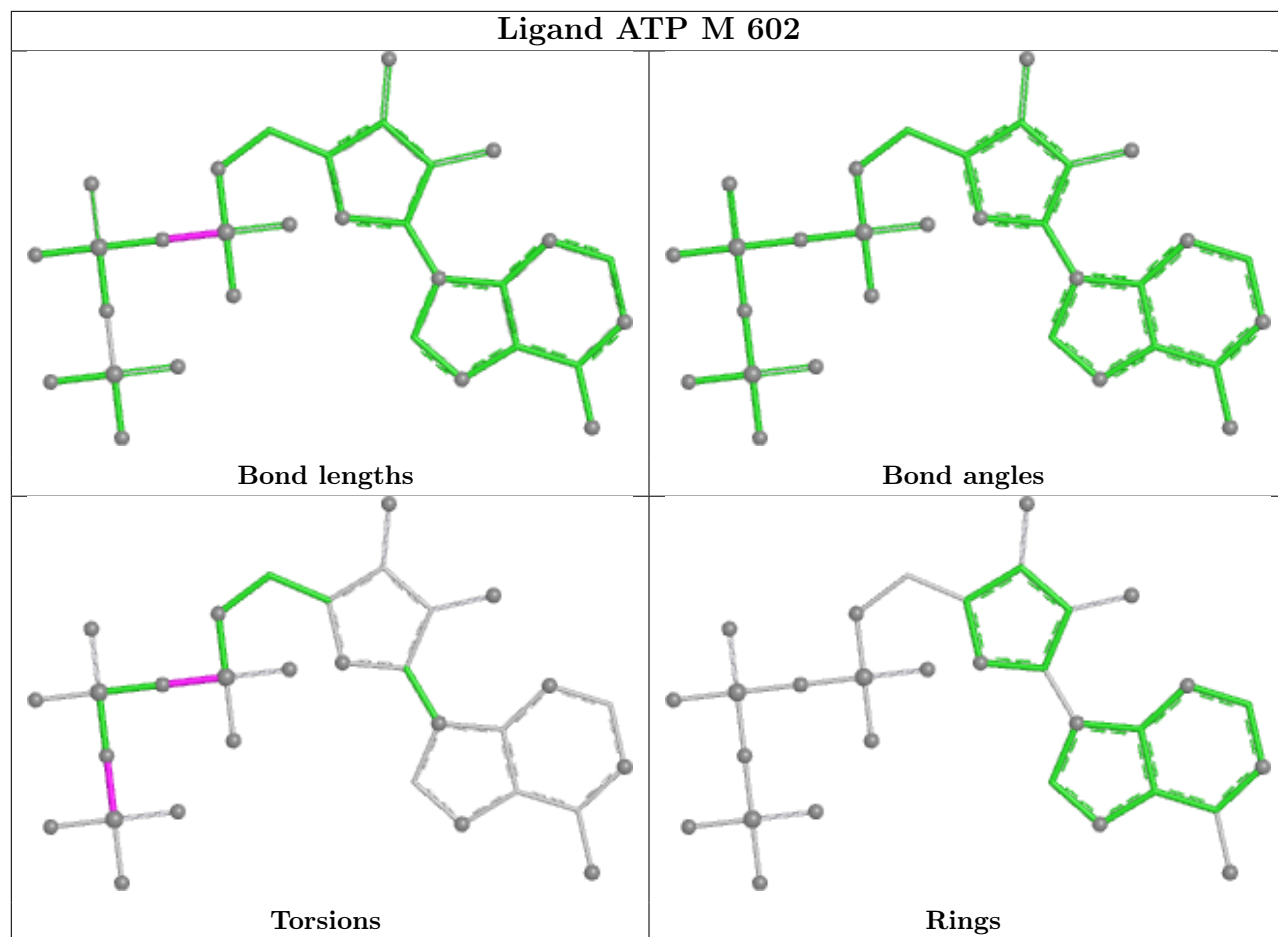
1 monomer is involved in 1 short contact:

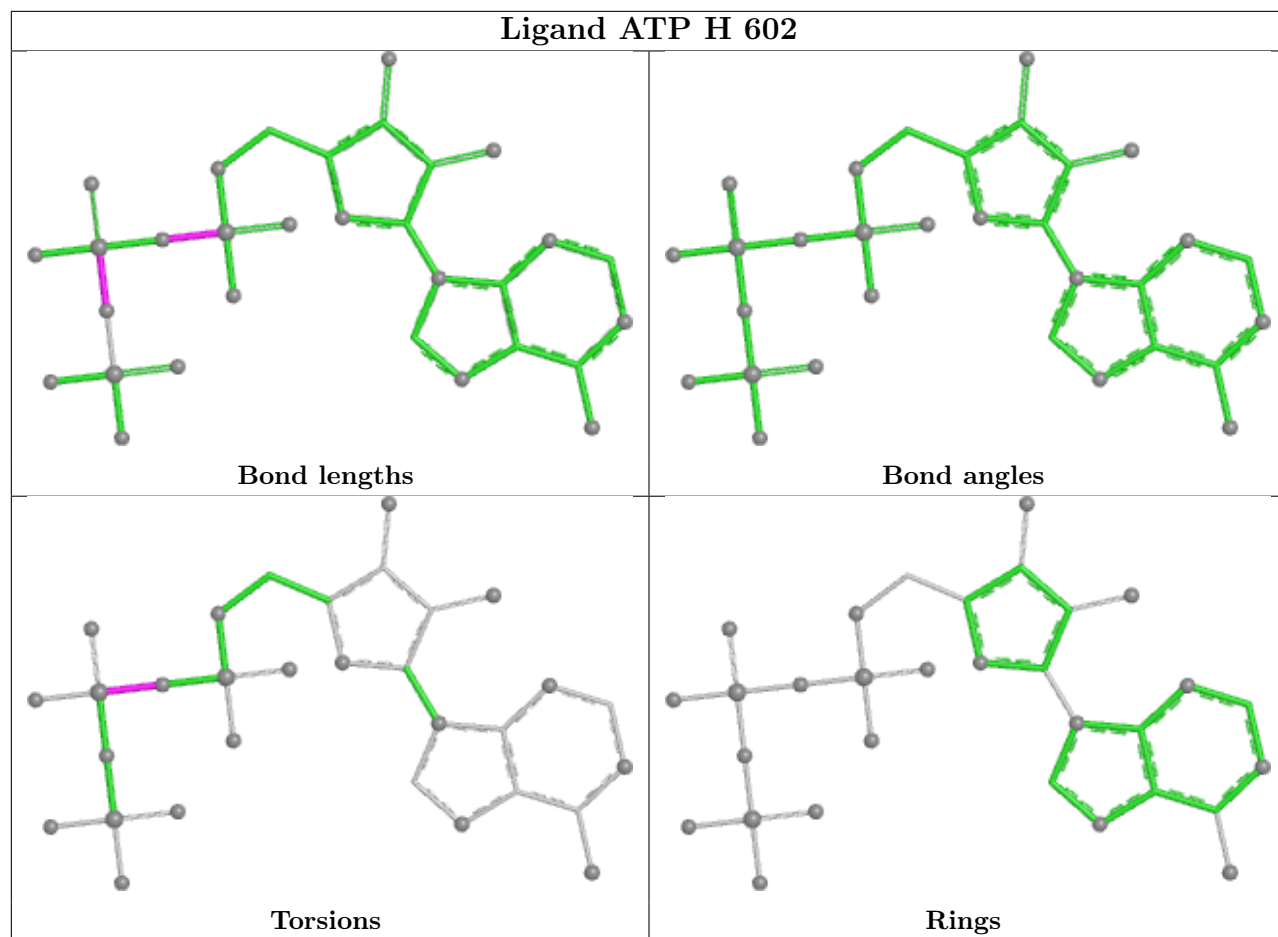
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 602 | ATP  | 1       | 0            |

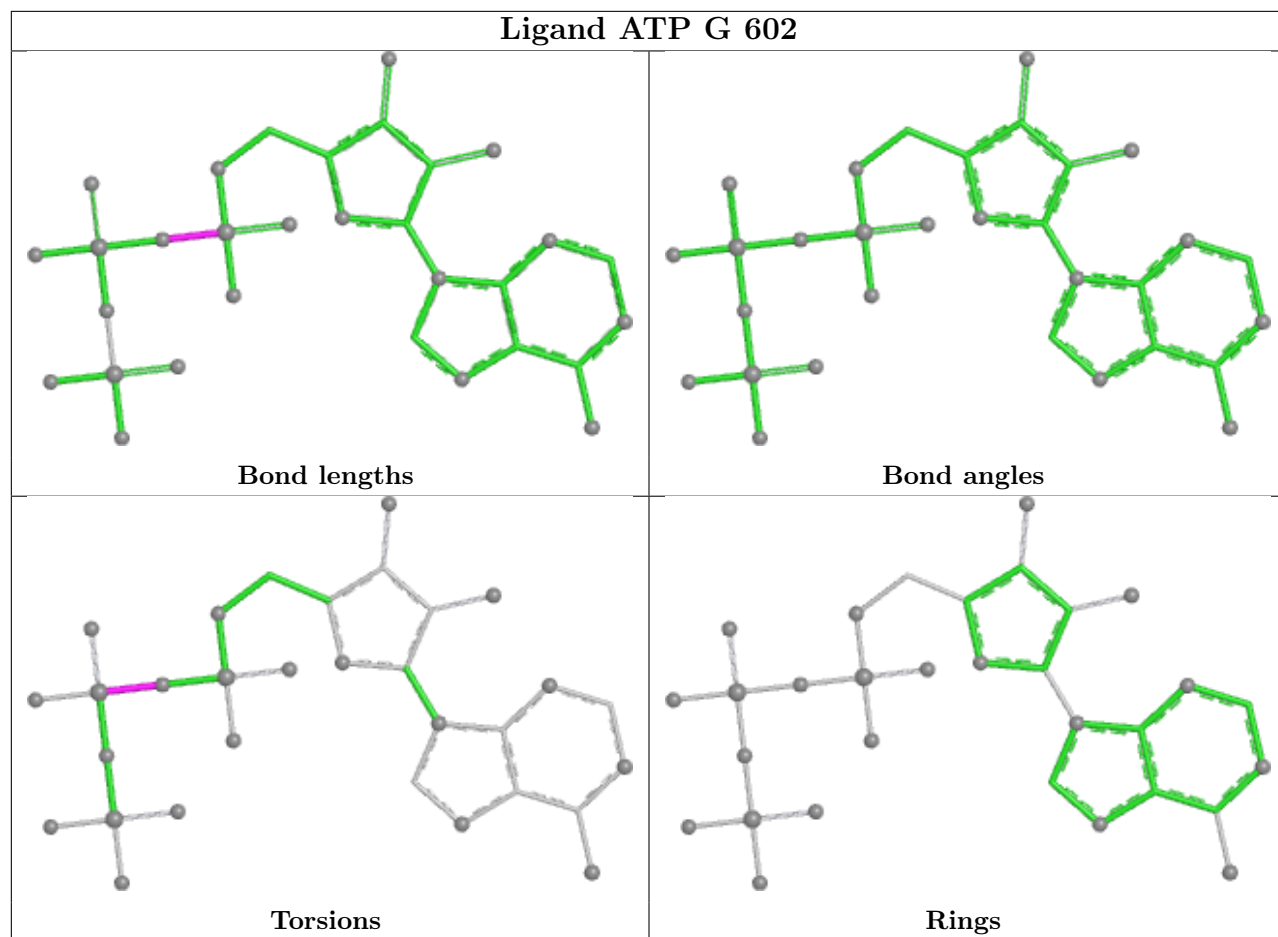
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

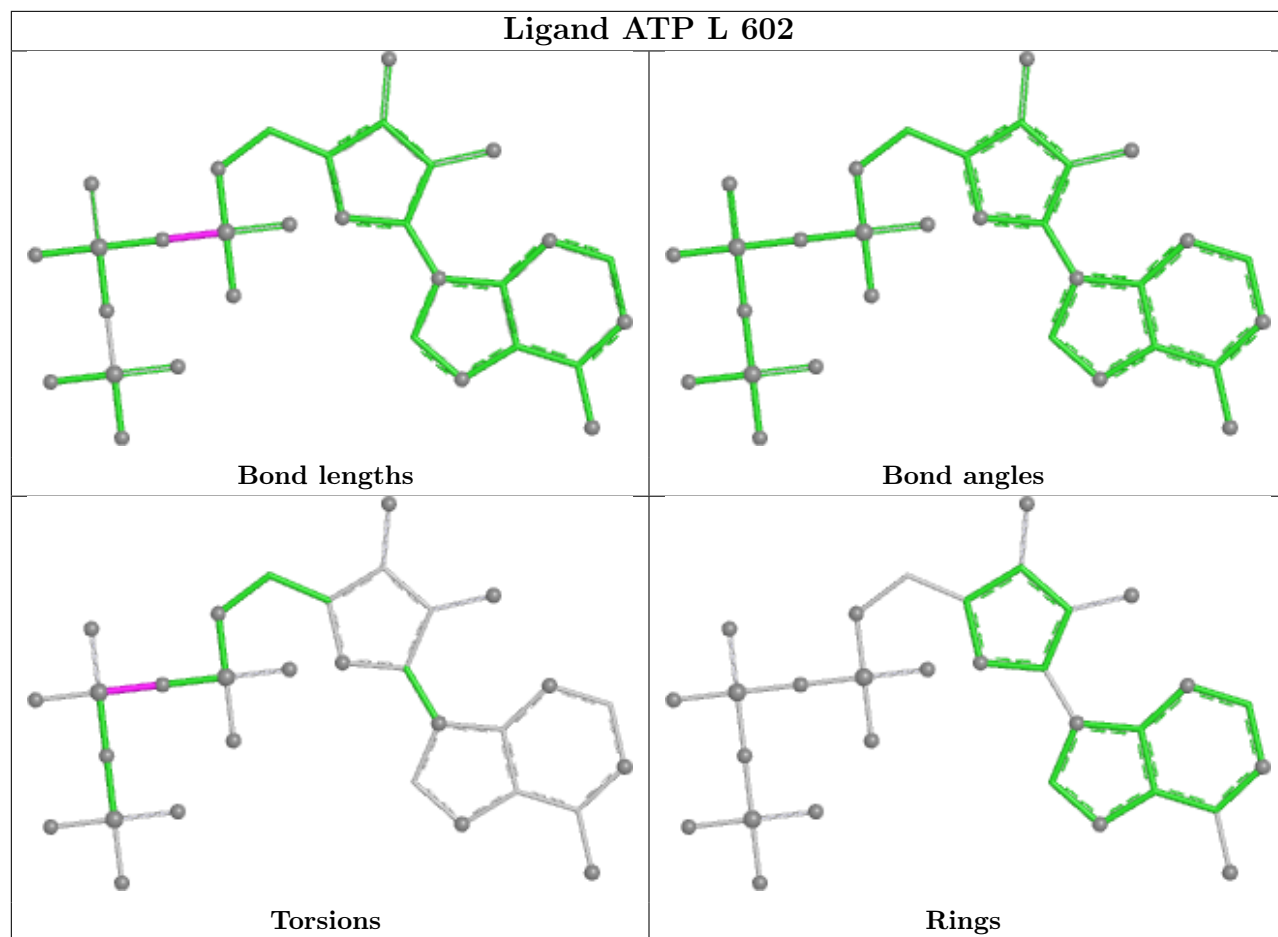


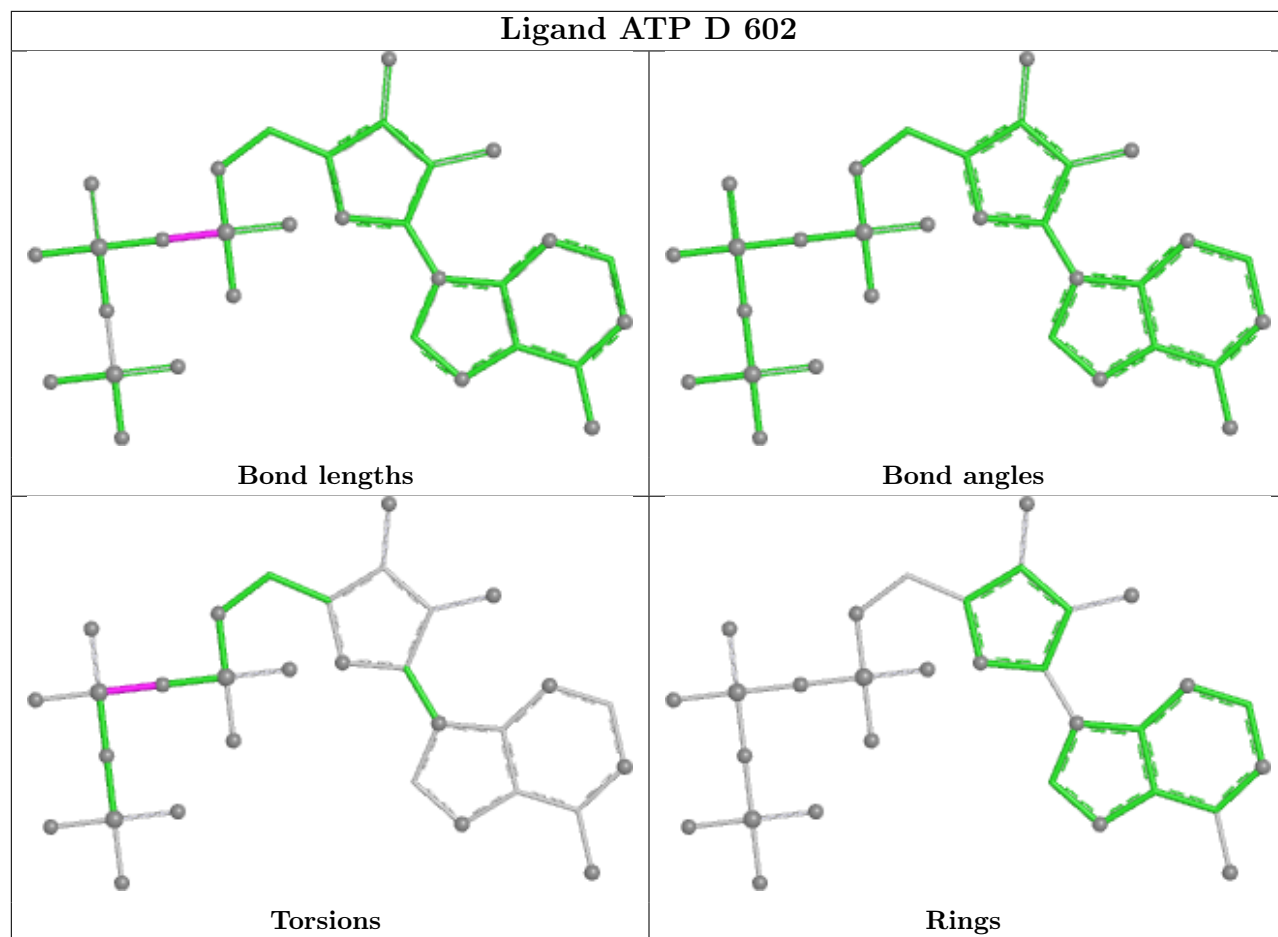


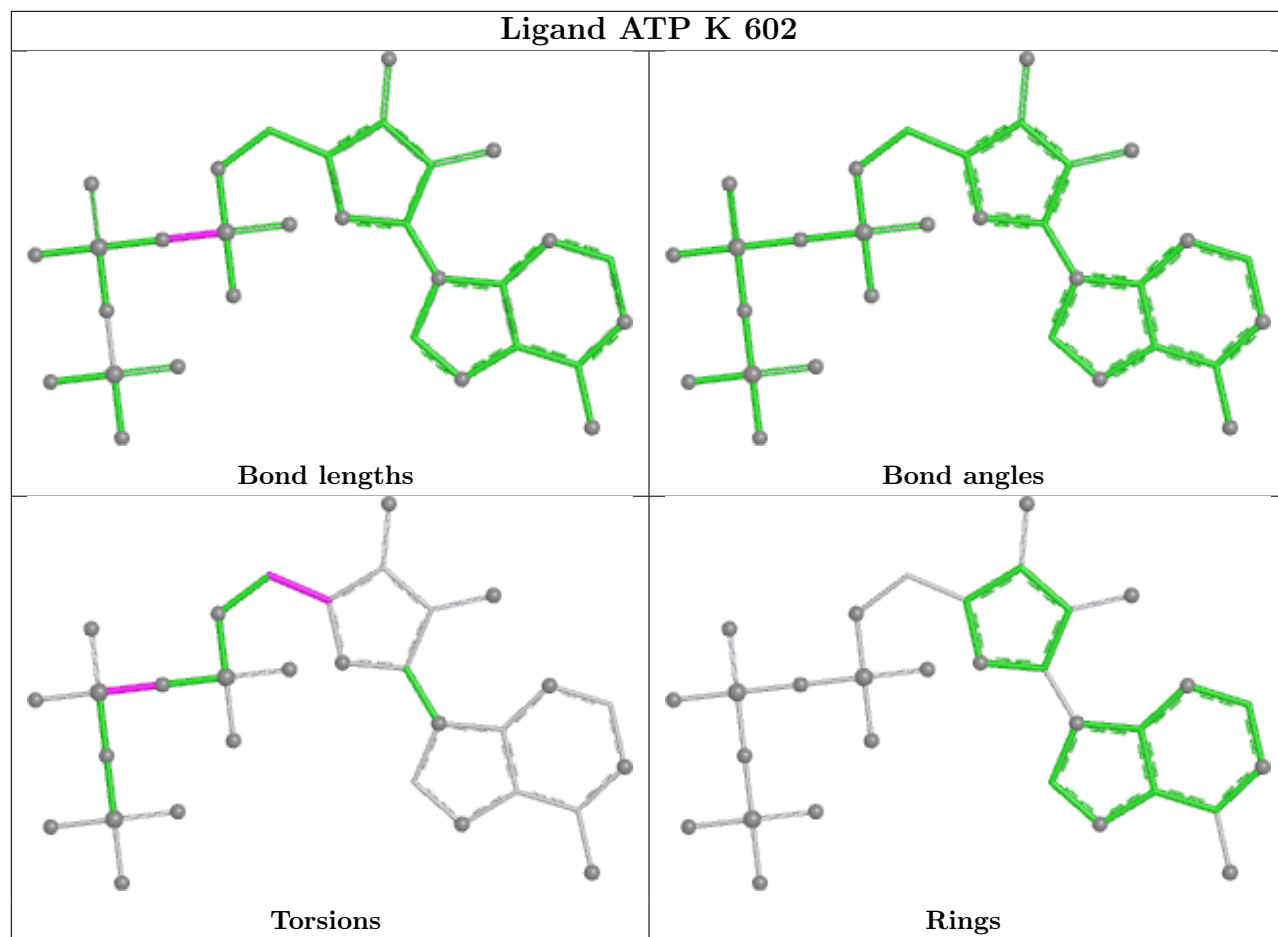


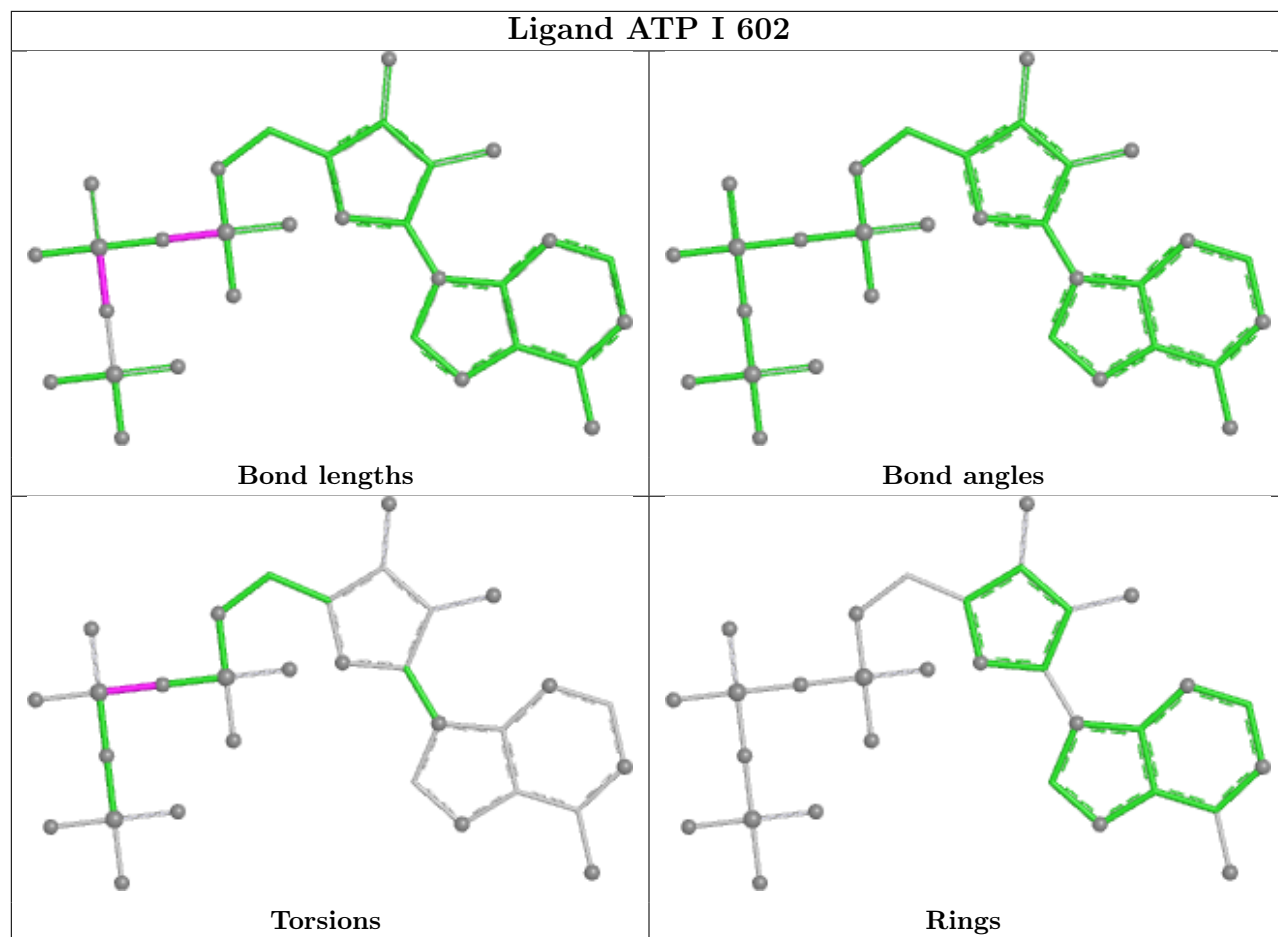


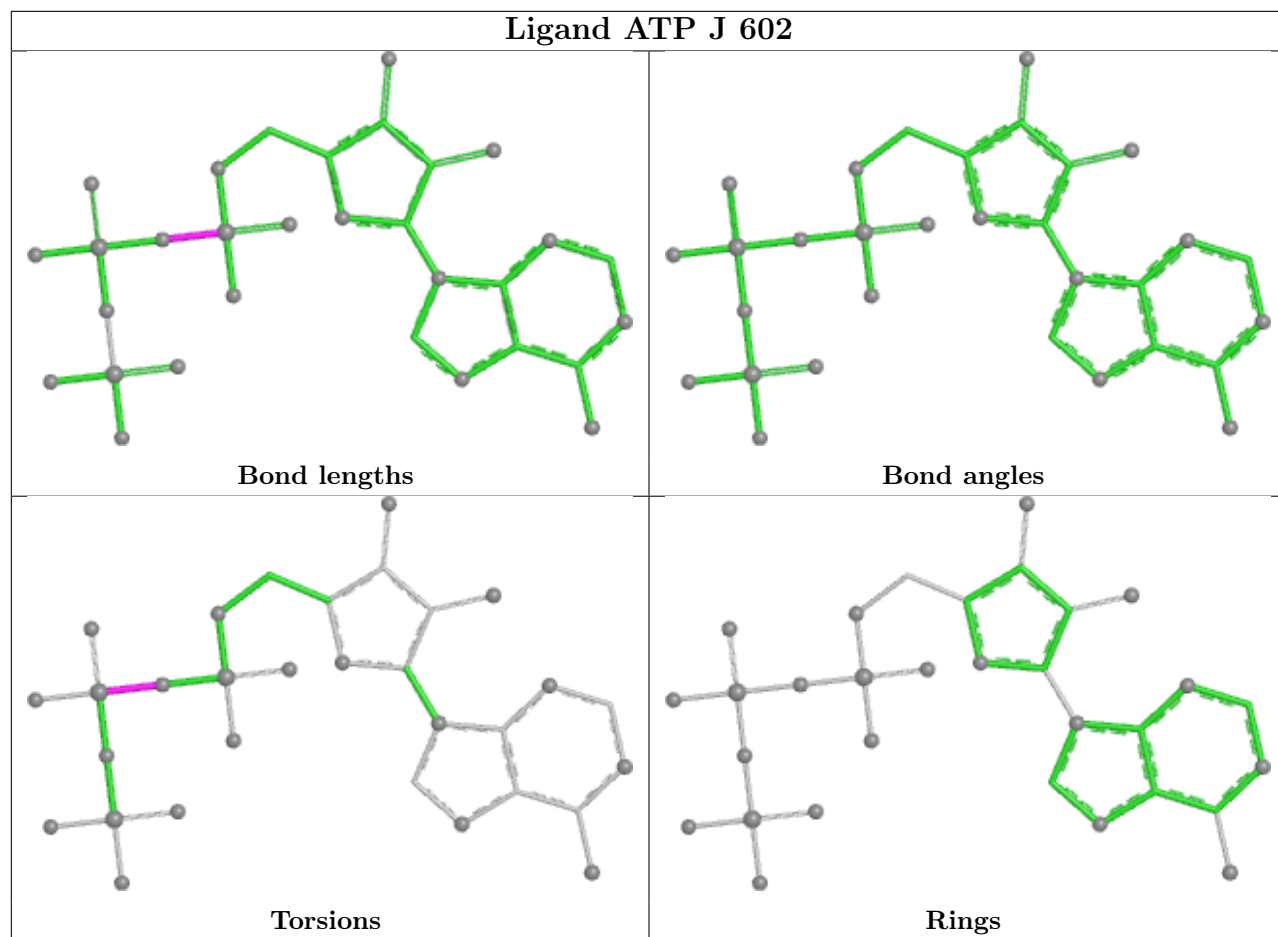




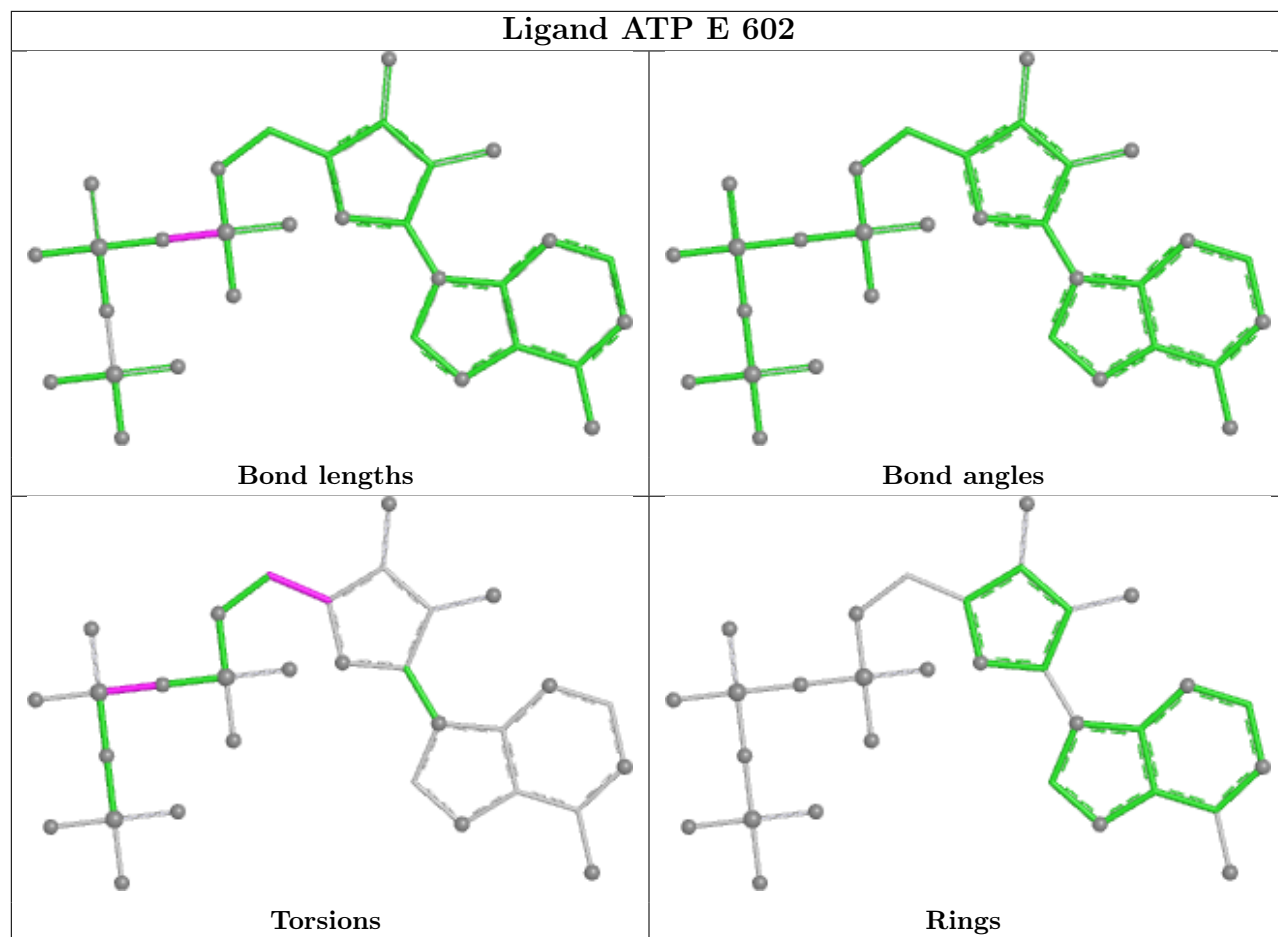


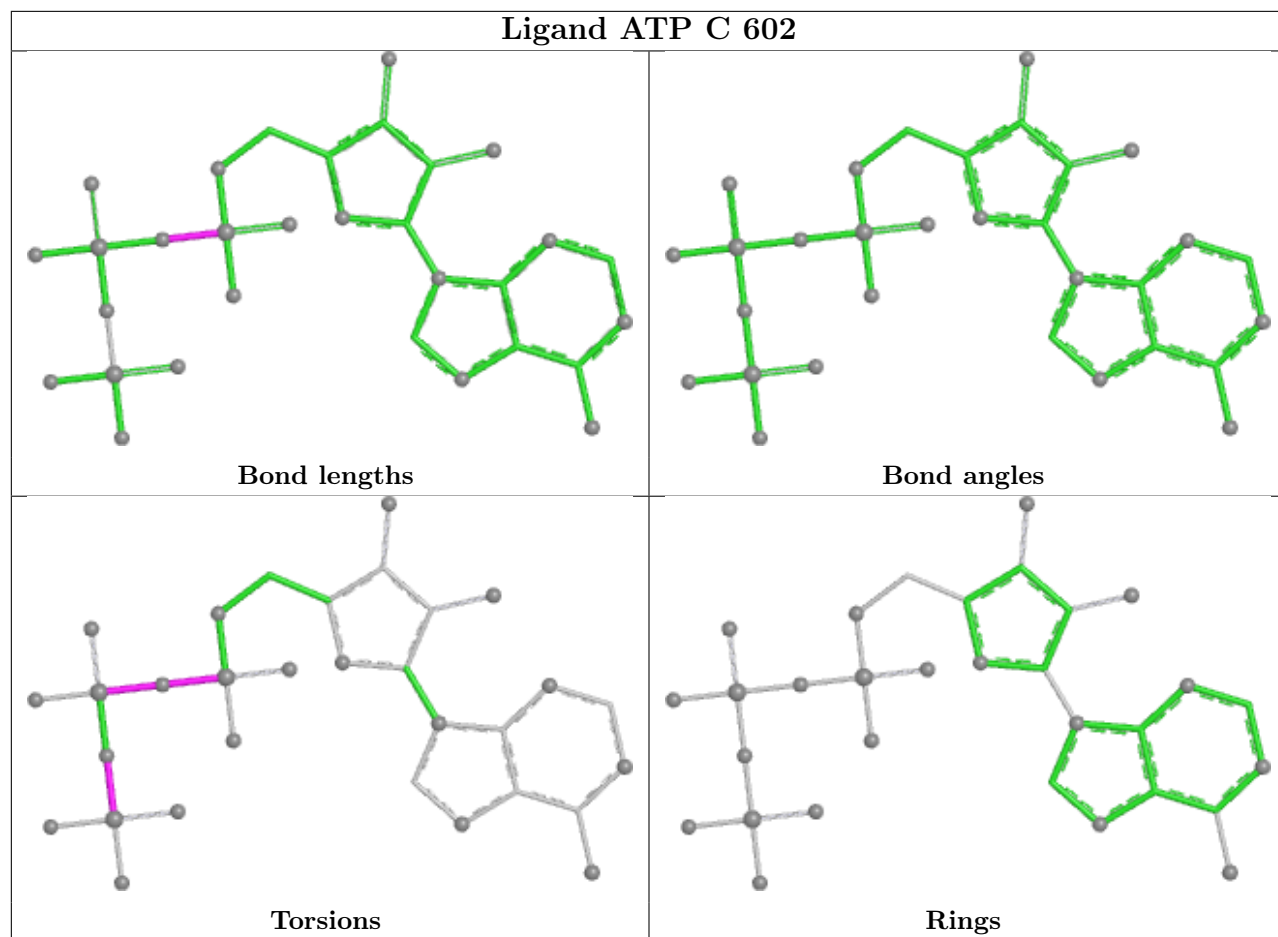




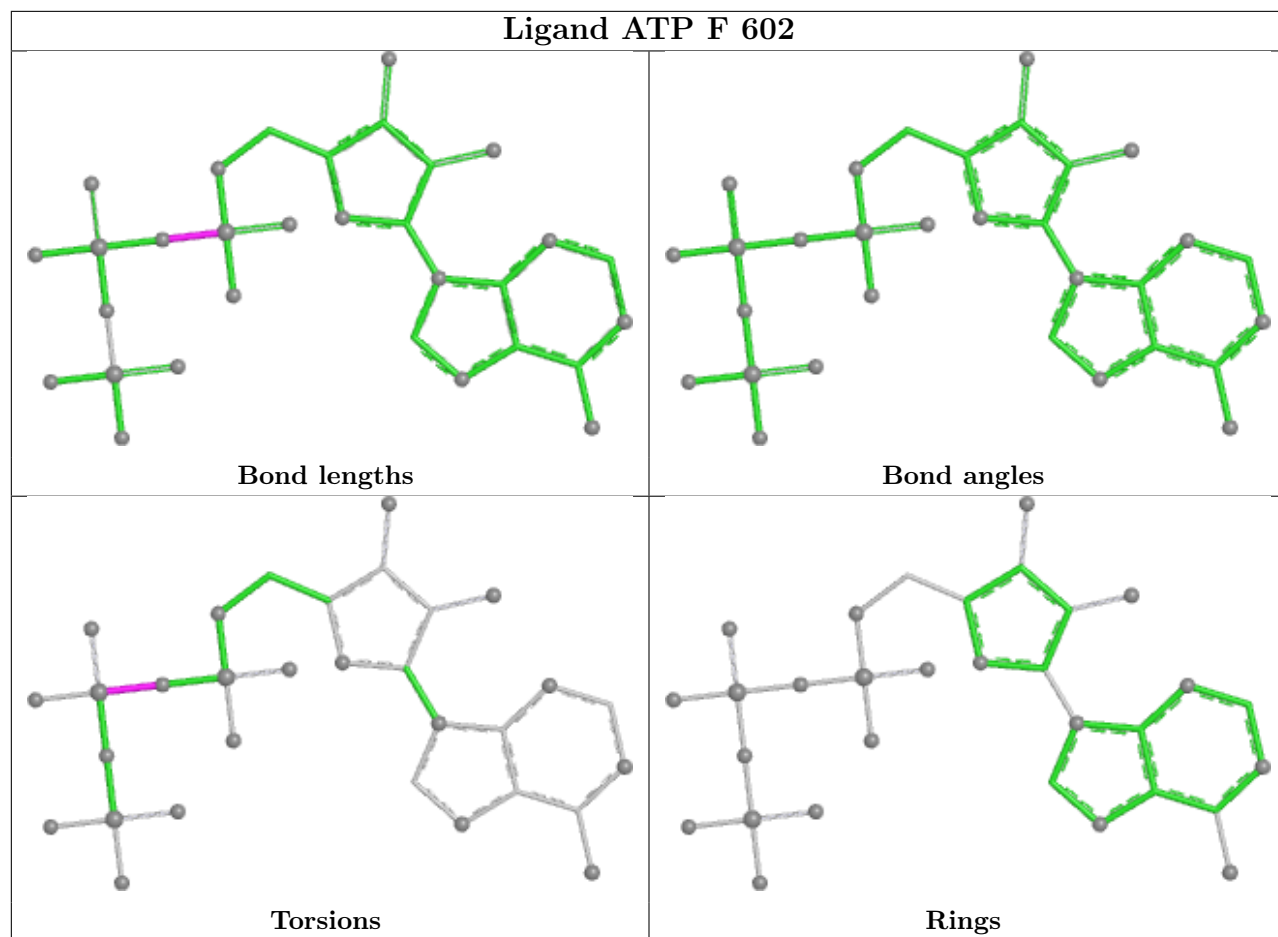


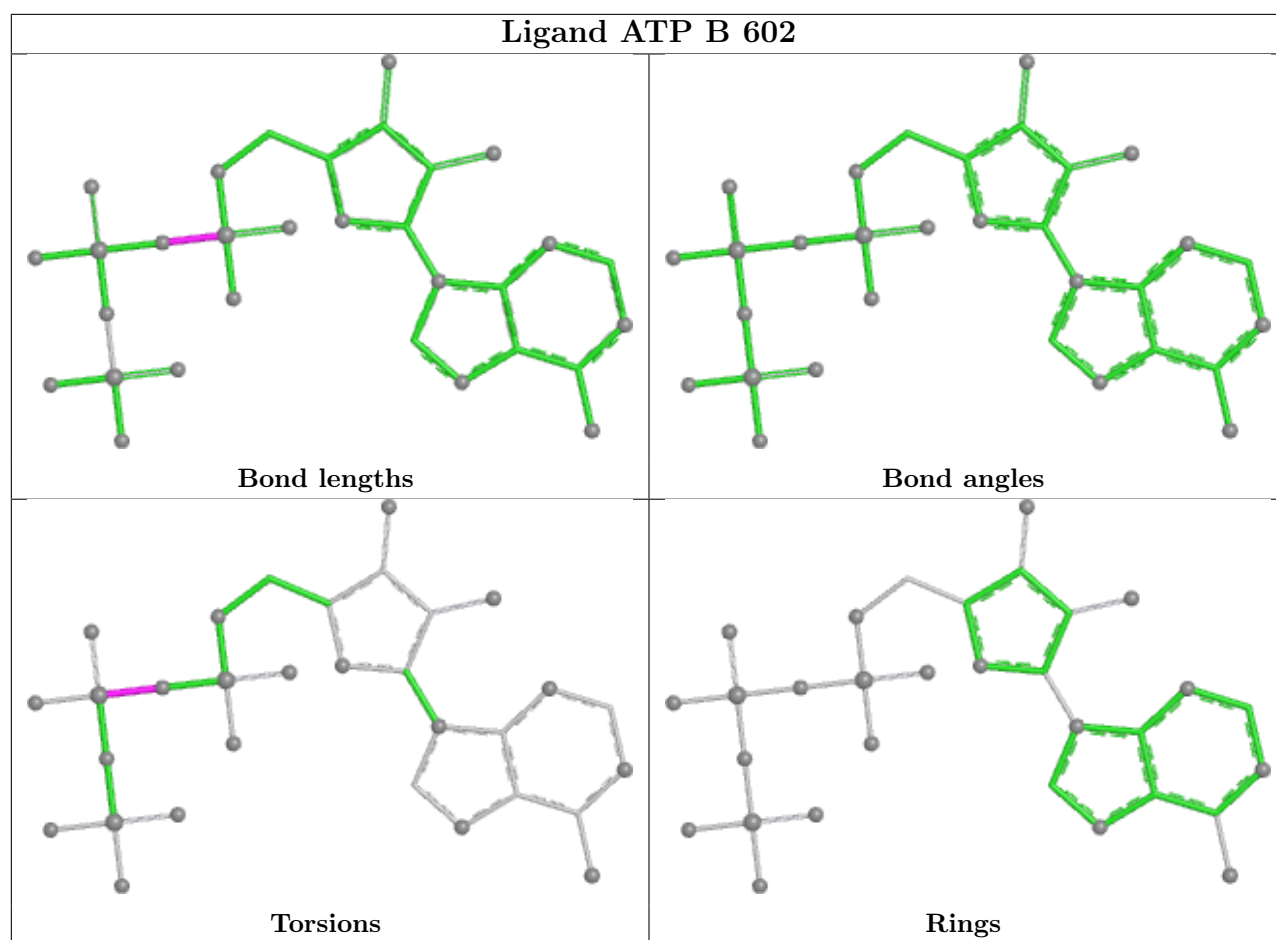
## Ligand ATP E 602





## Ligand ATP F 602





## 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.

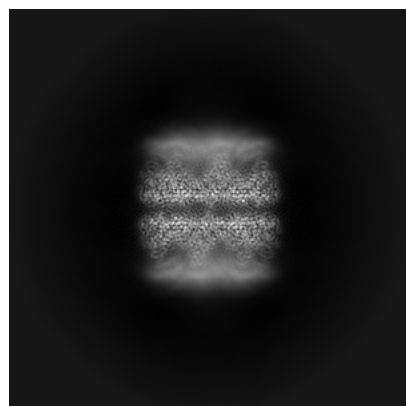
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16106. These allow visual inspection of the internal detail of the map and identification of artifacts.

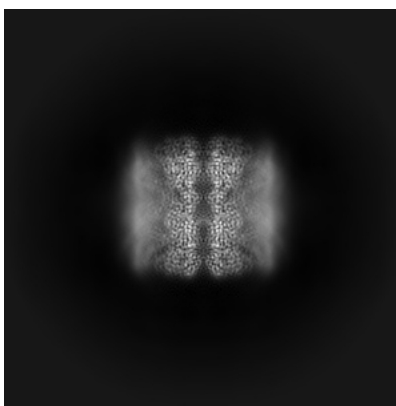
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

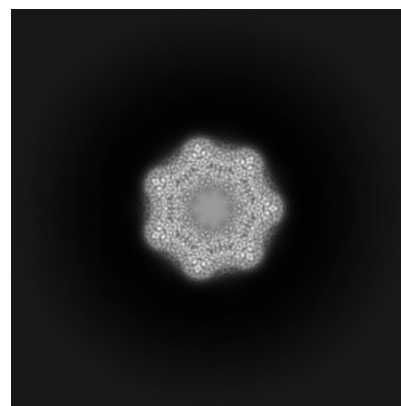
#### 6.1.1 Primary map



X

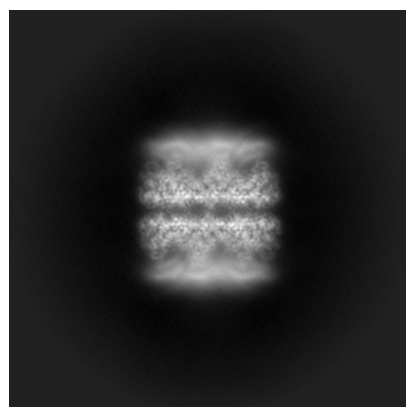


Y

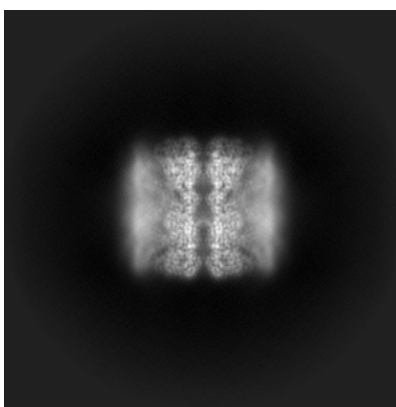


Z

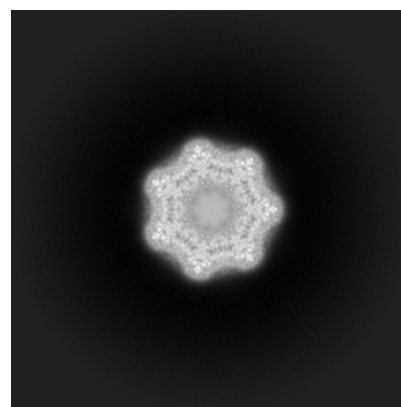
#### 6.1.2 Raw map



X



Y

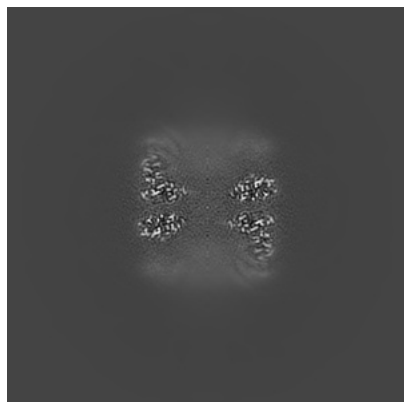


Z

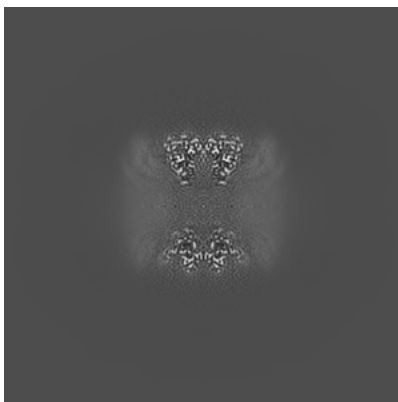
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

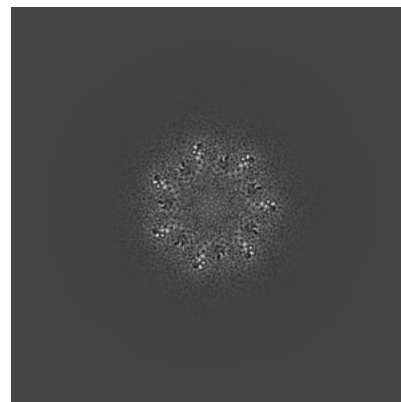
### 6.2.1 Primary map



X Index: 196

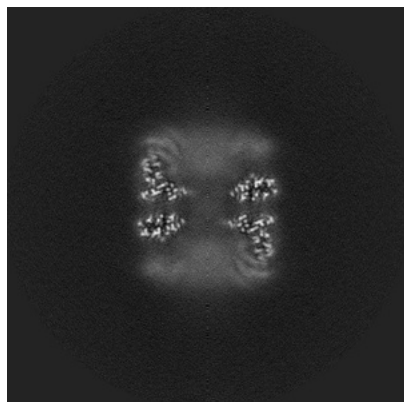


Y Index: 196

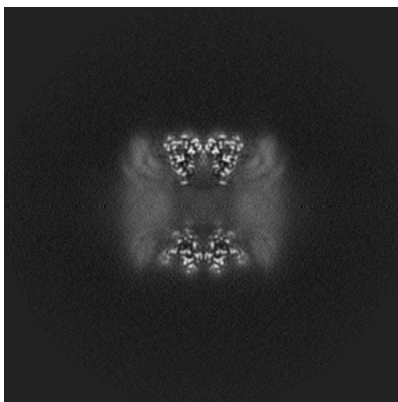


Z Index: 196

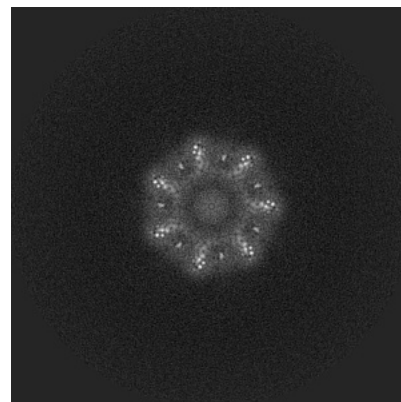
### 6.2.2 Raw map



X Index: 196



Y Index: 196

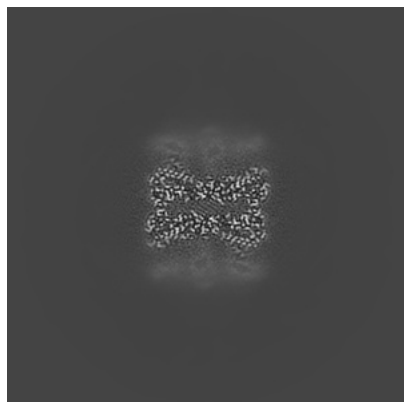


Z Index: 196

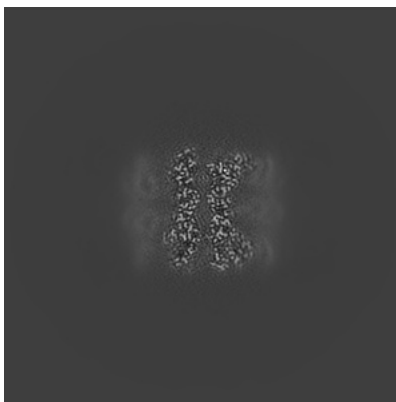
The images above show central slices of the map in three orthogonal directions.

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

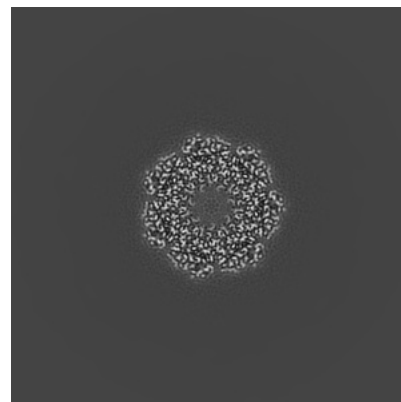
### 6.3.1 Primary map



X Index: 233

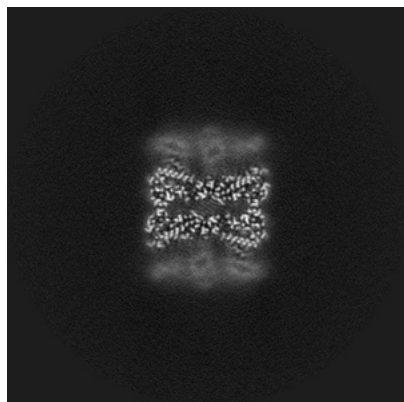


Y Index: 161

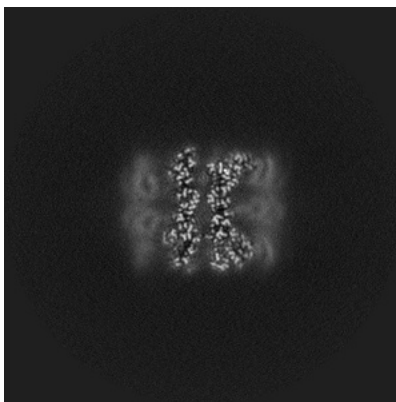


Z Index: 209

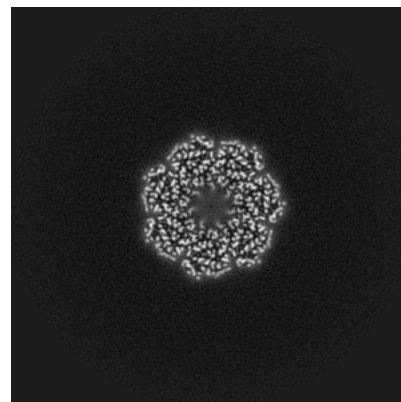
### 6.3.2 Raw map



X Index: 233



Y Index: 161

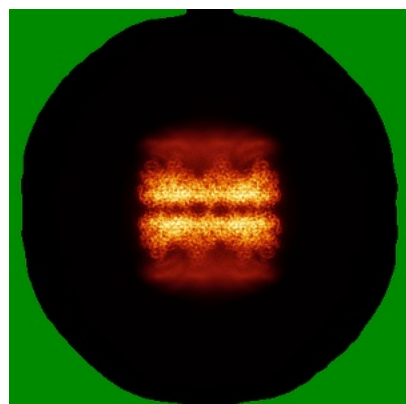


Z Index: 181

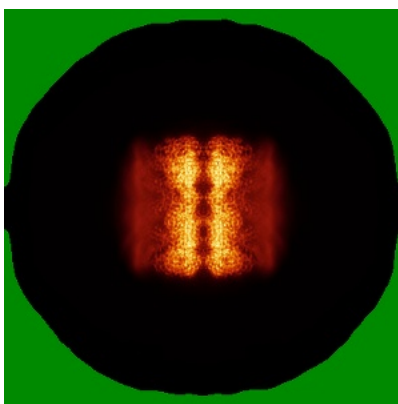
The images above show the largest variance slices of the map in three orthogonal directions.

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

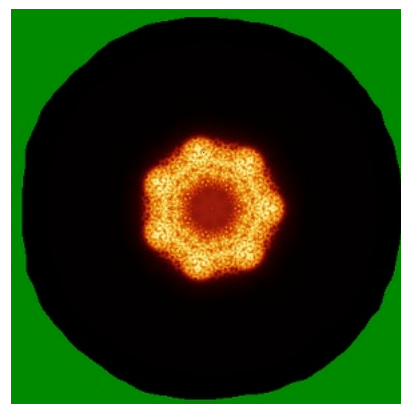
### 6.4.1 Primary map



X

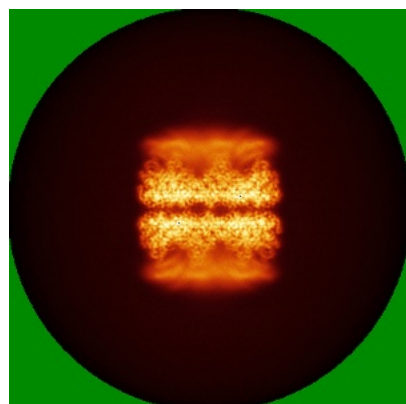


Y

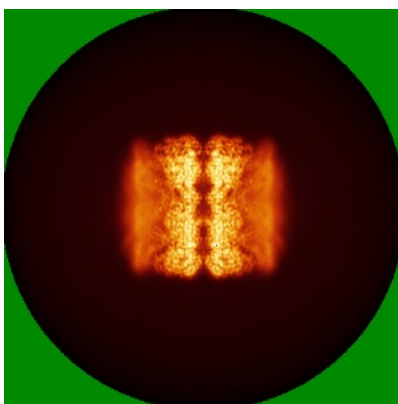


Z

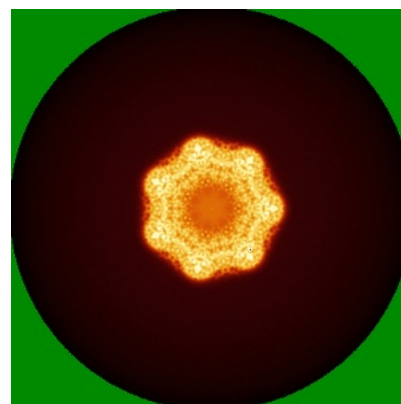
### 6.4.2 Raw map



X



Y

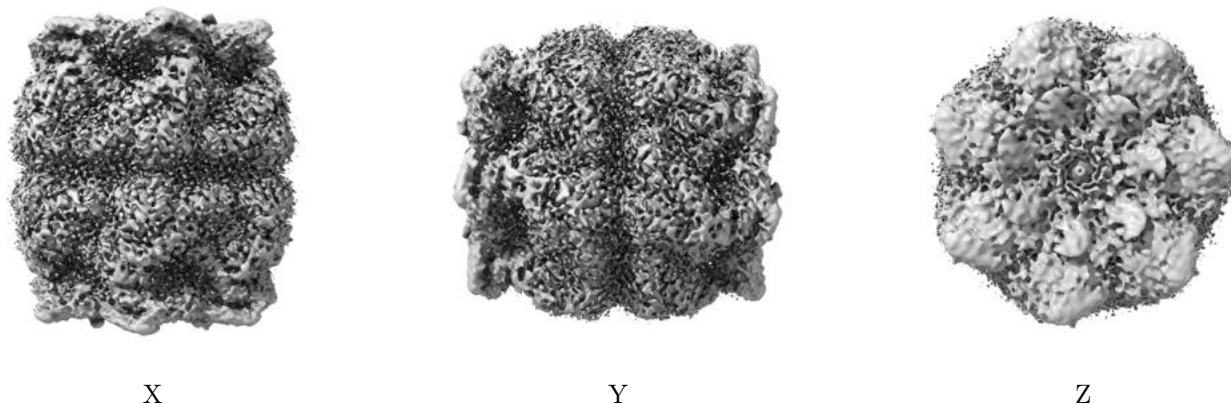


Z

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.

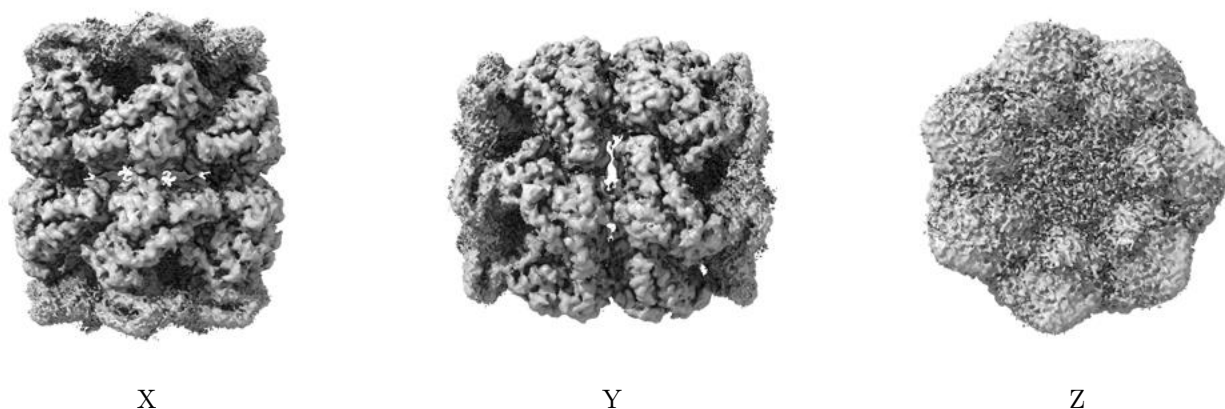
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

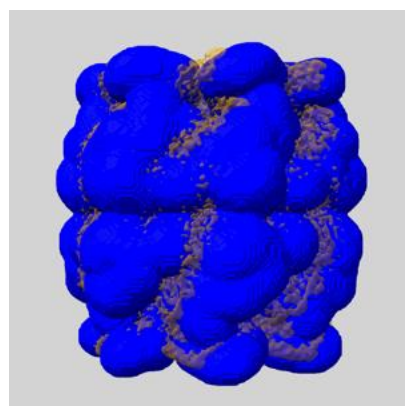
## 6.6 Mask visualisation [i](#)

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

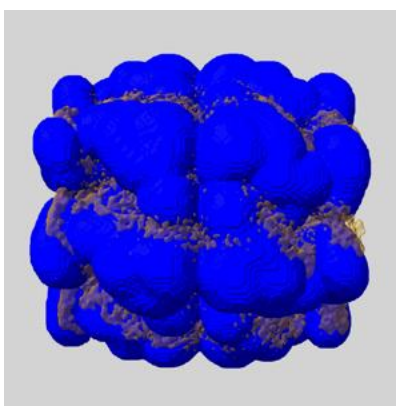
A mask typically either:

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

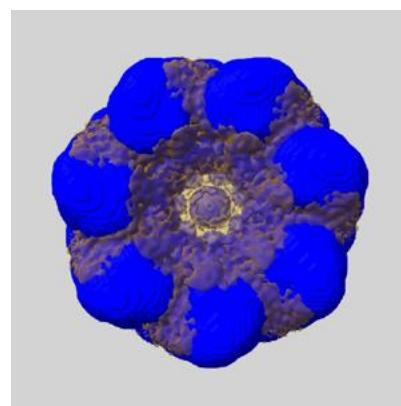
### 6.6.1 emd\_16106\_msk\_1.map [i](#)



X



Y

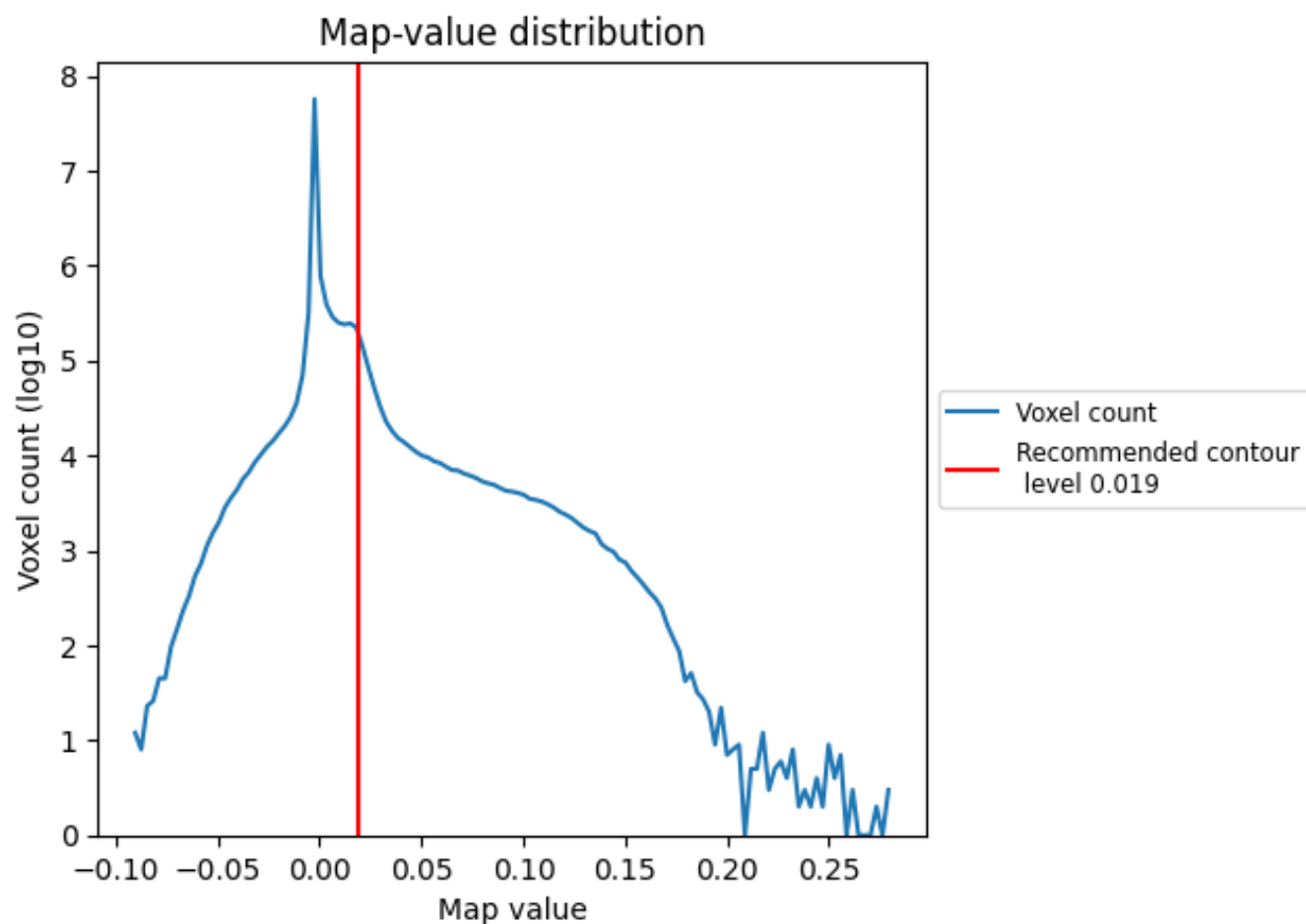


Z

## 7 Map analysis [i](#)

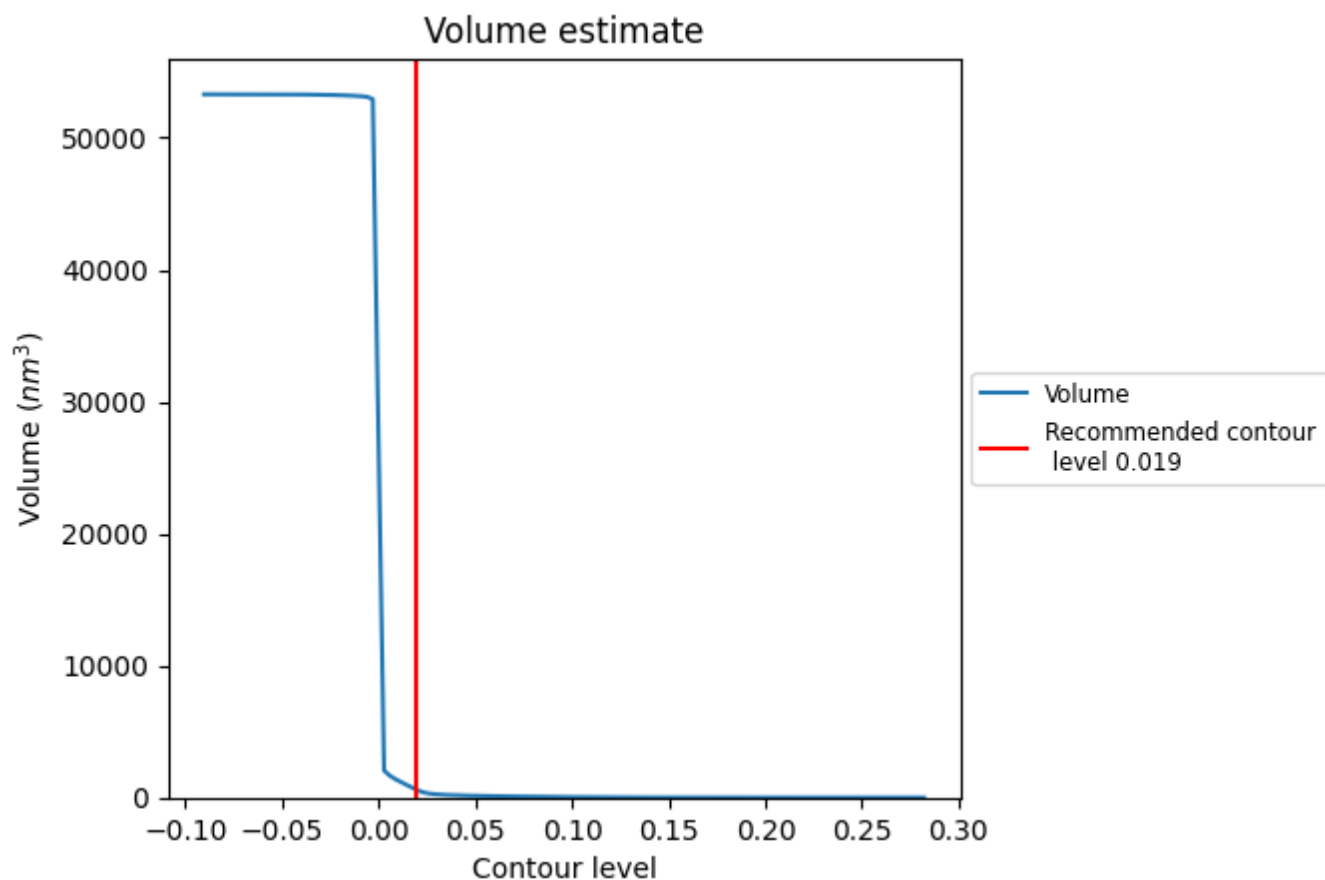
This section contains the results of statistical analysis of the map.

### 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.

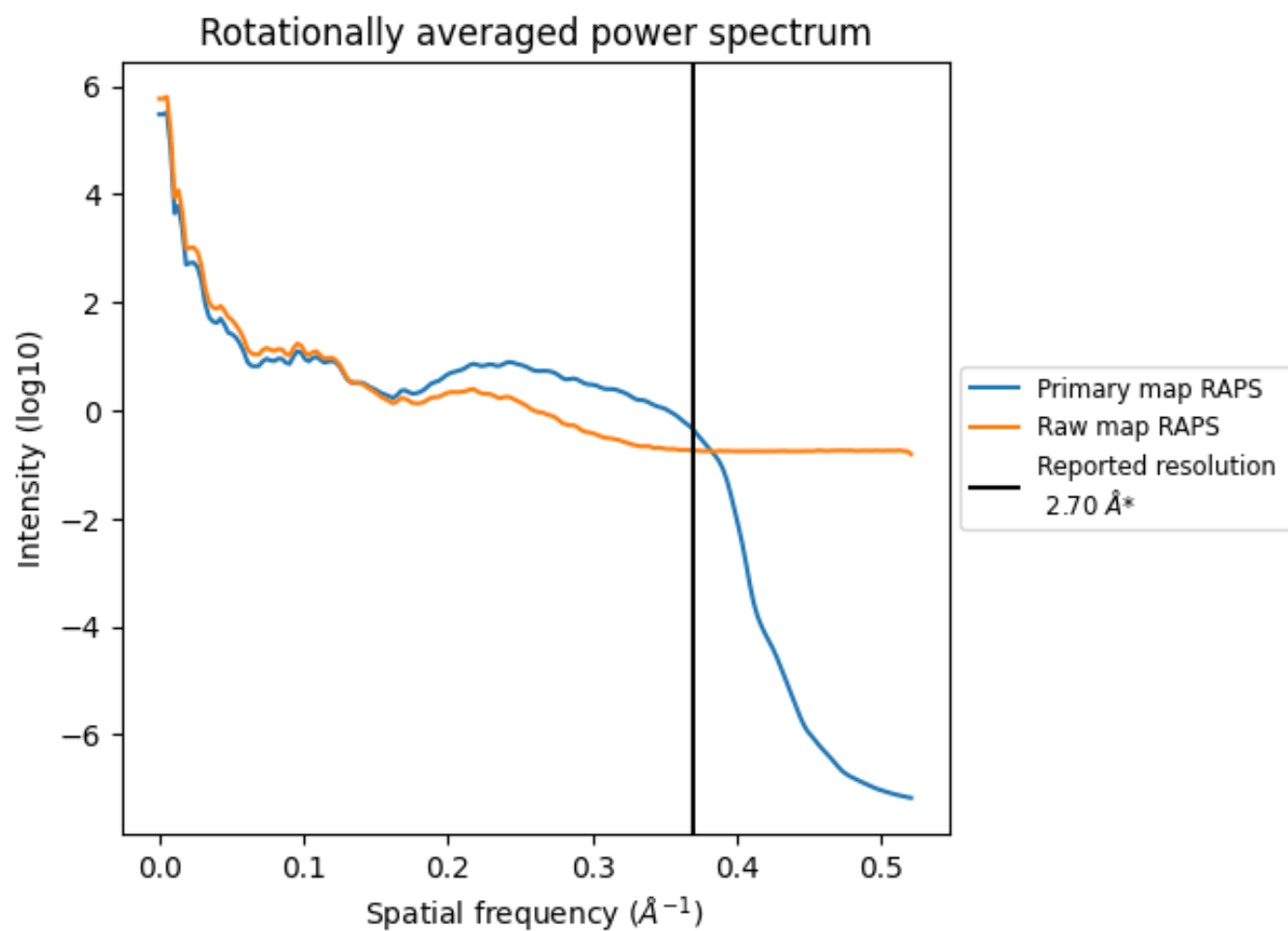
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 627  $\text{nm}^3$ ; this corresponds to an approximate mass of 566 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 ⓘ

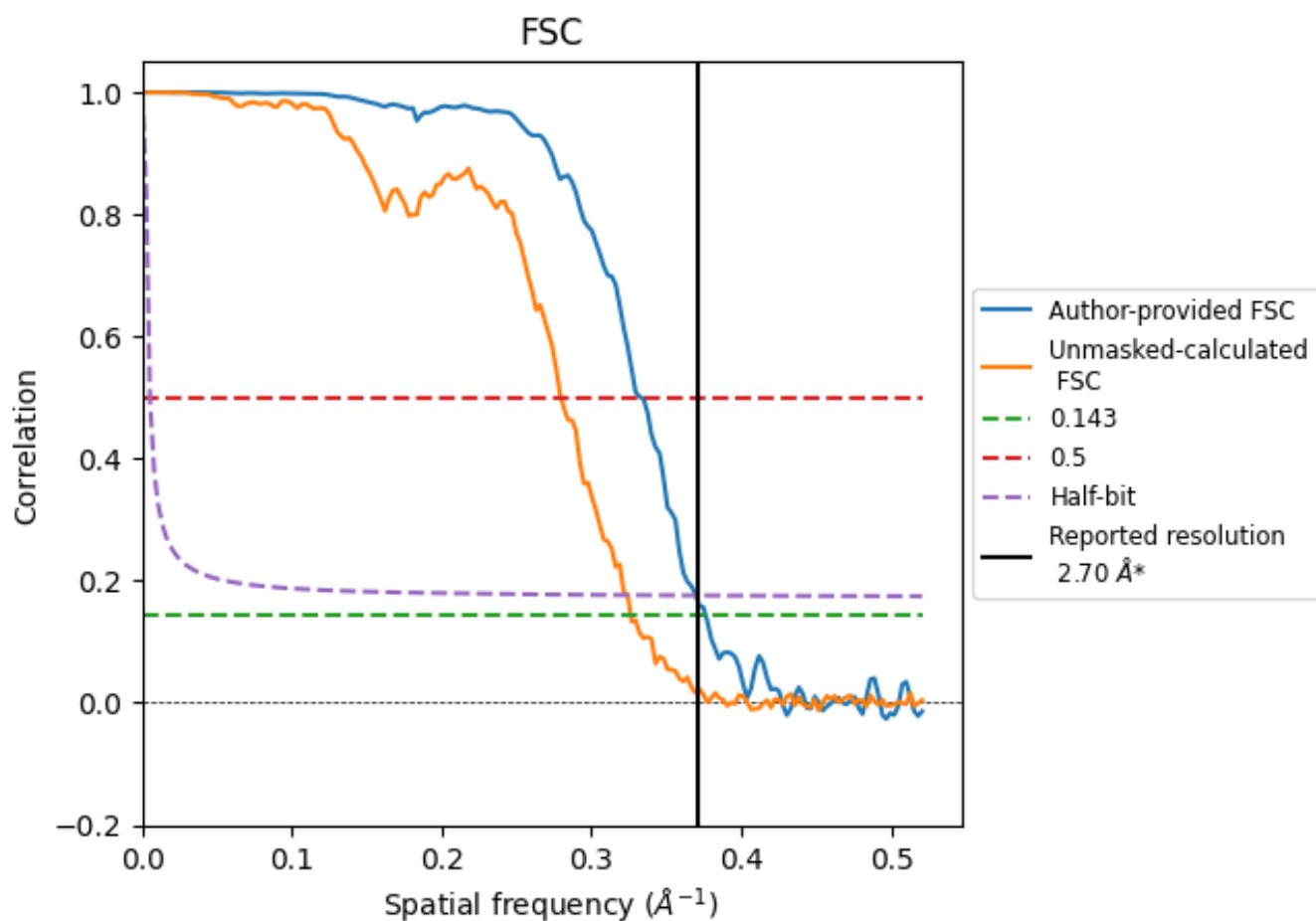


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

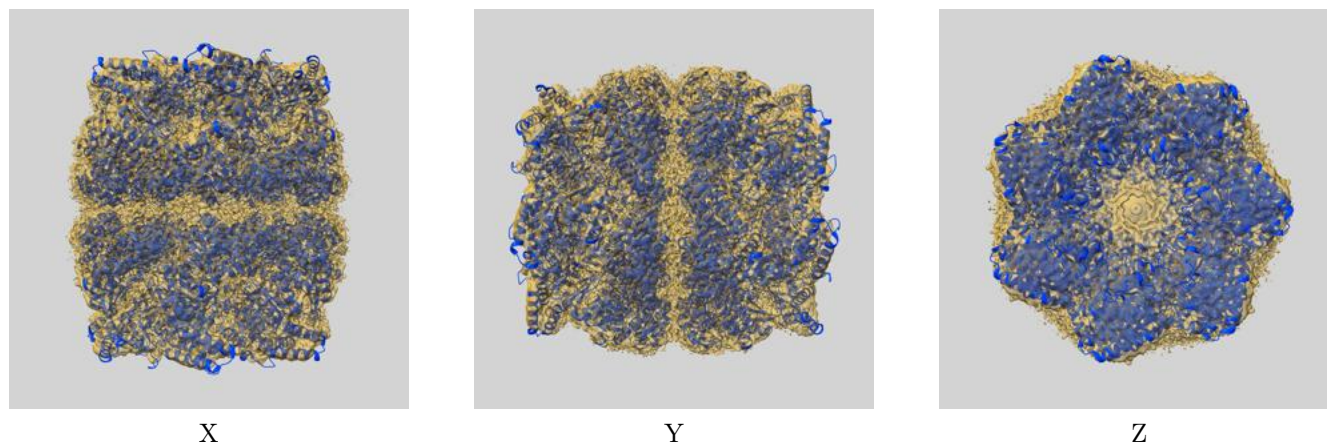
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.70                               | -    | -        |
| Author-provided FSC curve | 2.66                               | 3.00 | 2.70     |
| Unmasked-calculated*      | 3.06                               | 3.58 | 3.08     |

\*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 3.06 differs from the reported value 2.7 by more than 10 %

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

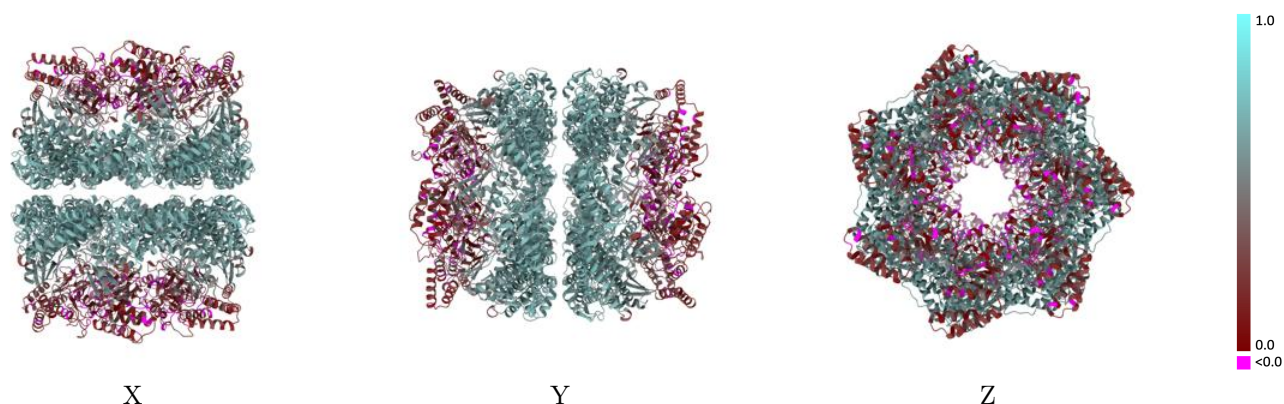
This section contains information regarding the fit between EMDB map EMD-16106 and PDB model 8BLC. Per-residue inclusion information can be found in section 3 on page 9.

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



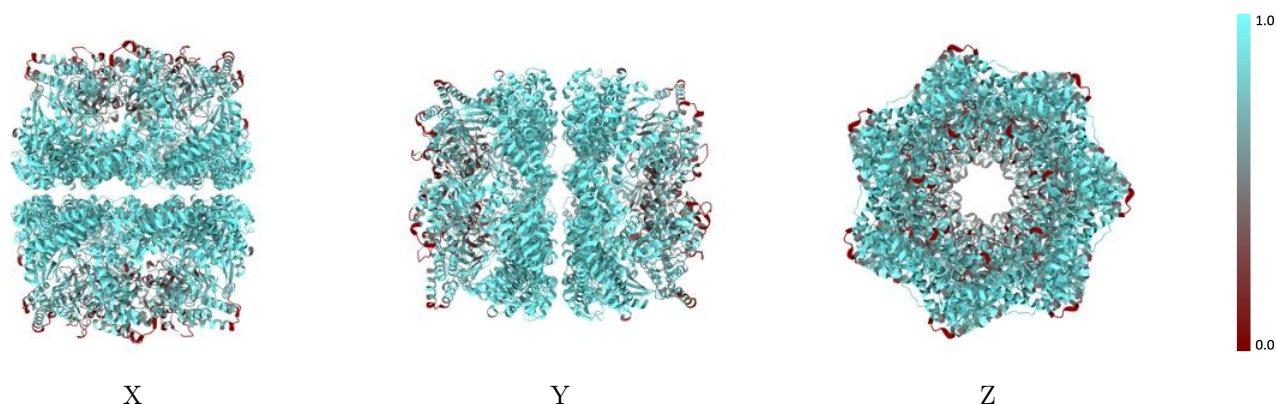
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



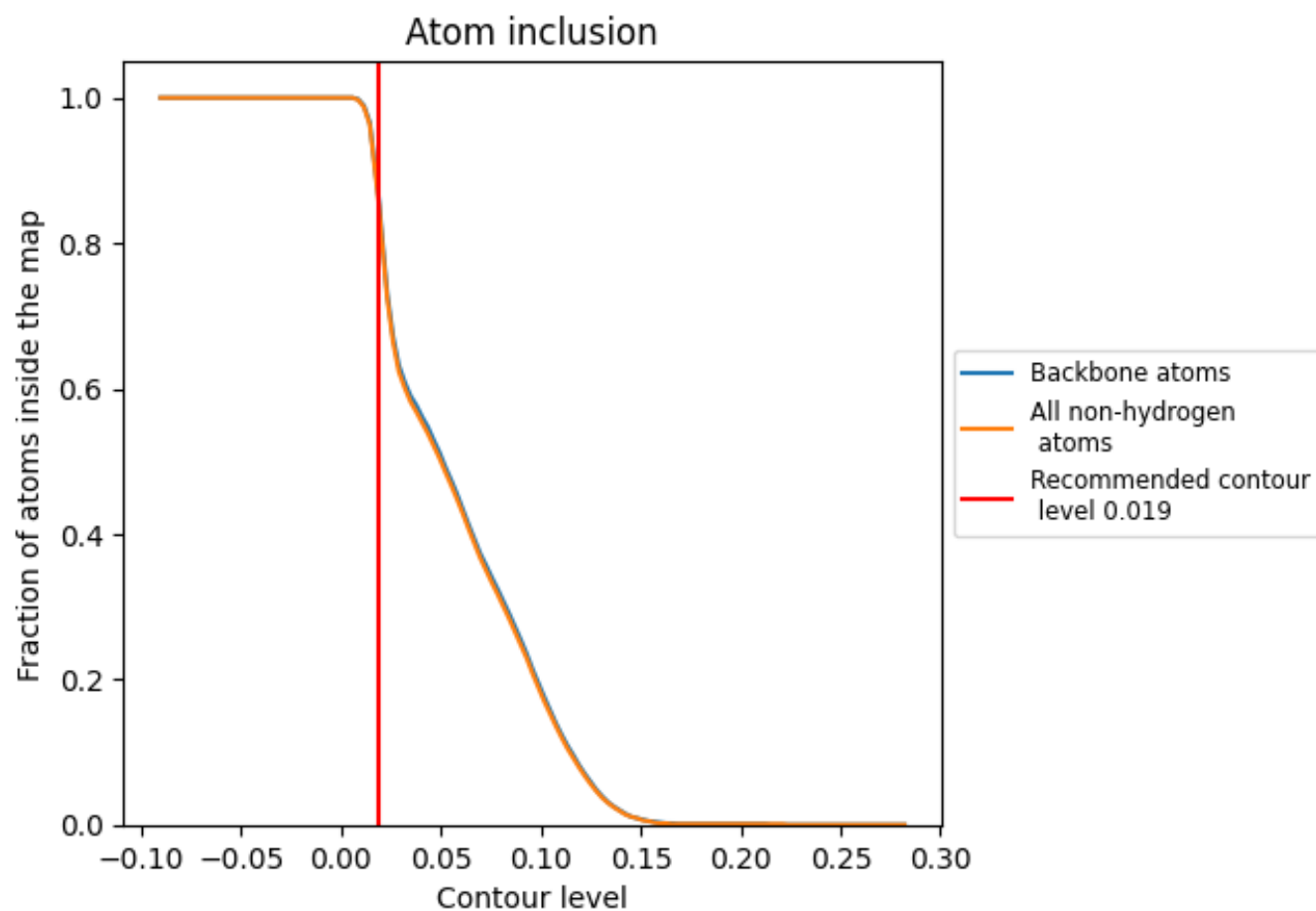
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.019) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8520 | <div><div></div></div> 0.4620 |
| A     | <div><div></div></div> 0.8550 | <div><div></div></div> 0.4630 |
| B     | <div><div></div></div> 0.8560 | <div><div></div></div> 0.4630 |
| C     | <div><div></div></div> 0.8550 | <div><div></div></div> 0.4630 |
| D     | <div><div></div></div> 0.8520 | <div><div></div></div> 0.4610 |
| E     | <div><div></div></div> 0.8530 | <div><div></div></div> 0.4620 |
| F     | <div><div></div></div> 0.8540 | <div><div></div></div> 0.4610 |
| G     | <div><div></div></div> 0.8520 | <div><div></div></div> 0.4620 |
| H     | <div><div></div></div> 0.8560 | <div><div></div></div> 0.4630 |
| I     | <div><div></div></div> 0.8510 | <div><div></div></div> 0.4610 |
| J     | <div><div></div></div> 0.8530 | <div><div></div></div> 0.4610 |
| K     | <div><div></div></div> 0.8500 | <div><div></div></div> 0.4610 |
| L     | <div><div></div></div> 0.8560 | <div><div></div></div> 0.4620 |
| M     | <div><div></div></div> 0.8500 | <div><div></div></div> 0.4600 |
| N     | <div><div></div></div> 0.8570 | <div><div></div></div> 0.4630 |

1.0

0.0

<0.0